```
=> d his

     (FILE 'HOME' ENTERED AT 14:42:44 ON 09 SEP 2000)

     FILE 'HCAPLUS' ENTERED AT 14:43:07 ON 09 SEP 2000
L1           222 S SHAN J?/AU
L2          6308 S WU X?/AU
L3           400 S LING L?/AU
L4           389 S PANG P?/AU
L5             1 S L1 AND L2 AND L3 AND L4
                 SELECT RN L5 1

     FILE 'REGISTRY' ENTERED AT 14:44:19 ON 09 SEP 2000
L6             12 S E1-12  12 cpds in L5 cite

     FILE 'HCAPLUS' ENTERED AT 14:44:33 ON 09 SEP 2000
L7             1 S L5 AND L6   1 cite w/ 12 cpds displayed
L8          7284 S L1-4
L9             1 S L8 AND HYPERIC?
L10            0 S L9 NOT L7

     FILE 'REGISTRY' ENTERED AT 14:47:00 ON 09 SEP 2000
L11              STR  55954-61-5  parent STR
L12           12 S L11
L13          183 S L11 FUL  183 cpds
                 SAVE L13 MEL572P/A

     FILE 'REGISTRY' ENTERED AT 14:50:03 ON 09 SEP 2000

     FILE 'HCAPLUS' ENTERED AT 14:53:35 ON 09 SEP 2000
L14          513 S L13  513 cites for L13
L15          136 S L14(L)THU/RL  <- 136 cites are linked to a therapeutic role
L16          214 S T-TYPE CALCIUM CHANNEL
L17       292644 S DEPRESSION OR HEART FAILURE OR CHF OR ISCHAEM? OR ISCHEM? OR
L18            1 S L15 AND L16
L19           12 S L15 AND L17
L20           12 S L19 OR L18
L21           11 S L20 NOT L7   11 cites related to a claimed use

     FILE 'REGISTRY' ENTERED AT 15:04:14 ON 09 SEP 2000

     FILE 'STNGUIDE' ENTERED AT 15:08:20 ON 09 SEP 2000

     FILE 'REGISTRY' ENTERED AT 15:14:15 ON 09 SEP 2000
L22              STR 147593-87-1
L23           11 S L22 SSS SAM SUB=L13
L24          148 S L22 SSS FUL SUB=L13  148 cpds based on cl 2
                 SAVE L24 MEL572S1/A

     FILE 'HCAPLUS' ENTERED AT 15:38:09 ON 09 SEP 2000
L25          510 S L24   510 cites

     FILE 'REGISTRY' ENTERED AT 15:39:01 ON 09 SEP 2000

     FILE 'STNGUIDE' ENTERED AT 15:39:56 ON 09 SEP 2000

     FILE 'REGISTRY' ENTERED AT 15:51:44 ON 09 SEP 2000
L26              STR  55954-61-5
L27              STR L26
L28              STR L26
L29              STR L28
L30            2 S L26-29 SSS SAM SUB=L24
L31           36 S L26-29 SSS FUL SUB=L24  36 cpds based on A-D provisos of cl 18
                 SAVE L31 MEL572S2/A

     FILE 'HCAPLUS' ENTERED AT 16:04:49 ON 09 SEP 2000
L32          476 S L31

     FILE 'REGISTRY' ENTERED AT 16:05:19 ON 09 SEP 2000
```

inventor search

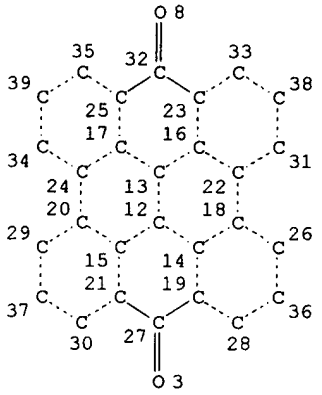
112 cpds after subtracting cl18 A-D

compounds of L2

```
L33          112 S L24 NOT L31   ← A-D provisos of cl 18

     FILE 'HCAPLUS' ENTERED AT 16:05:59 ON 09 SEP 2000
L34           93 S L33           ← cites for remaing cpds
L35           10 S L34(L)THU/RL
                 SELECT RN L35 1-10   ← 10 cites related to a therapeutic role

     FILE 'REGISTRY' ENTERED AT 16:12:46 ON 09 SEP 2000
L36           65 S E13-77
L37           75 S L6 OR L36     > these are all the cpds displayed so far;
L38           93 S L33 NOT L37   ← these cpds are subtracted to avoid
                                   repetative hits
     FILE 'HCAPLUS' ENTERED AT 16:13:46 ON 09 SEP 2000
L39           68 S L38           68 cites for L38

     FILE 'REGISTRY' ENTERED AT 16:16:11 ON 09 SEP 2000
L40              STR L29
L41              STR L40        > subset str for E & F of cl.18
L42            1 S L40 OR L41 SSS FUL  SUB=L24   1 cpd for D or E
L43           93 S L38 NOT L42   still 93 cpds after subtracting
L44              STR L22                                          set
L45            9 S L44 SSS SAM SUB=L24
L46          128 S L44 SSS FUL SUB=L24   ← cpds for cl 20   out L42

     FILE 'HCAPLUS' ENTERED AT 16:33:32 ON 09 SEP 2000

     FILE 'REGISTRY' ENTERED AT 16:40:37 ON 09 SEP 2000
L47          105 S L46 NOT L37

     FILE 'HCAPLUS' ENTERED AT 16:40:57 ON 09 SEP 2000

     FILE 'REGISTRY' ENTERED AT 16:42:47 ON 09 SEP 2000
L48           77 S L47 NOT L31   ← 77 cpds for cl 20 after subtracting out
                                   previously displayed cps
     FILE 'HCAPLUS' ENTERED AT 16:43:11 ON 09 SEP 2000
L49           63 S L48           63 cites
L50            1 S L49 AND PY>1999
L51           62 S L49 NOT L50   62 cites w/ pub year < 2000
L52            0 S L51 AND (L16 OR L17)
L53            1 S L51(L)THU/RL   1 cite linked to therapy
L54           61 S L51 NOT L53   61 cites; 1-31 displayed; the remaining
                 SAVE L54 MEL572HC/L   cites are saved if you want them
```

=> d que l14

L11 STR



parent STR
all sites open to substn except 3, 8
this broad STR was used for the method claim in order to pick up possible 103's

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

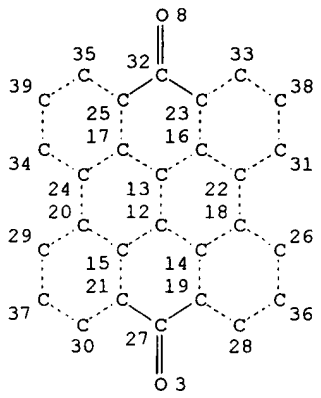
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE
L13 183 SEA FILE=REGISTRY SSS FUL L11
L14 513 SEA FILE=HCAPLUS ABB=ON PLU=ON L13

=> d que l25

L11 STR

parent STR

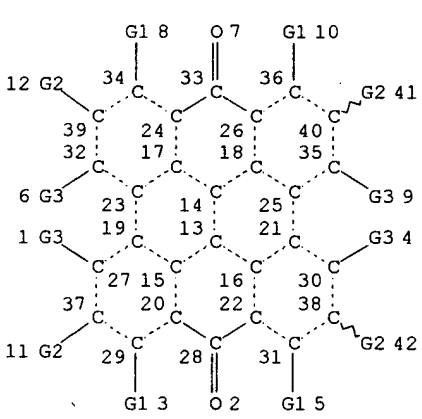


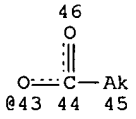
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

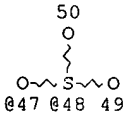
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

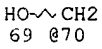
STEREO ATTRIBUTES: NONE
L13 183 SEA FILE=REGISTRY SSS FUL L11
L22 STR

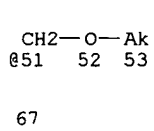
subset STR based on claim 2

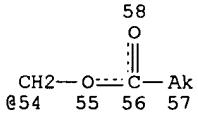


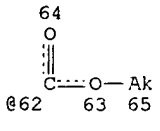




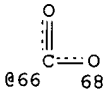








Page 1-A



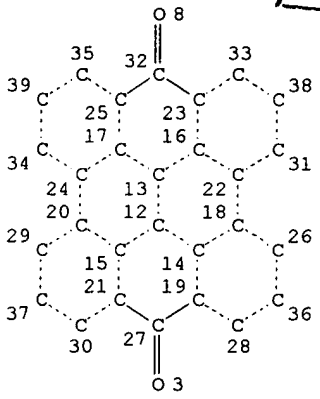
Page 2-A

```
VAR G1=H/OH/59/43
VAR G2=H/AK/X/47/48
VAR G3=H/AK/OH/59/43/70/51/54/62/66
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  68
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  69

STEREO ATTRIBUTES: NONE
L24          148 SEA FILE=REGISTRY SUB=L13 SSS FUL L22
L25          510 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24
```

this part of the search is to subtract out the provisos of cl. 18

=> d que 132

L11 STR parent STR

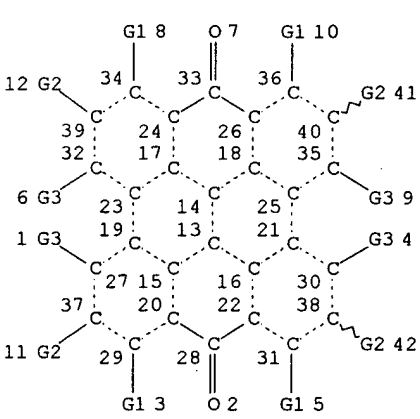


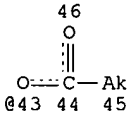
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

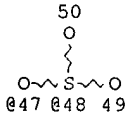
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

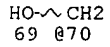
STEREO ATTRIBUTES: NONE
L13 183 SEA FILE=REGISTRY SSS FUL L11
L22 STR

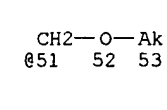
subset STR for claim 2

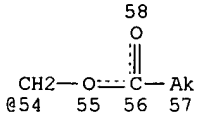


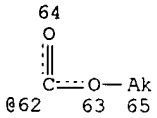




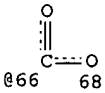








Page 1-A



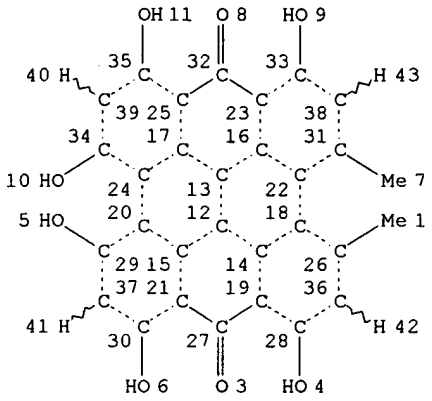
Page 2-A

VAR G1=H/OH/59/43
VAR G2=H/AK/X/47/48
VAR G3=H/AK/OH/59/43/70/51/54/62/66
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 68
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 69

these are the proviso subset STR's

STEREO ATTRIBUTES: NONE
L24 148 SEA FILE=REGISTRY SUB=L13 SSS FUL L22
L26 STR

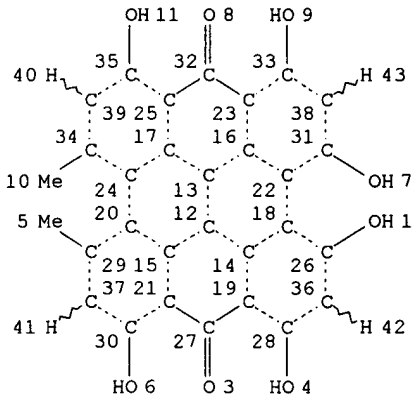


"A"

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
L27 STR



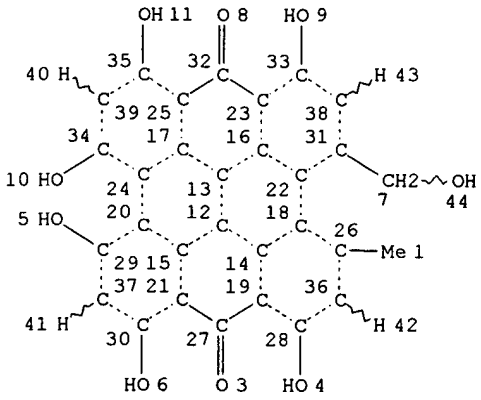
"B"

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 42

more proviso substrs for claim 18

STEREO ATTRIBUTES: NONE
L28 STR

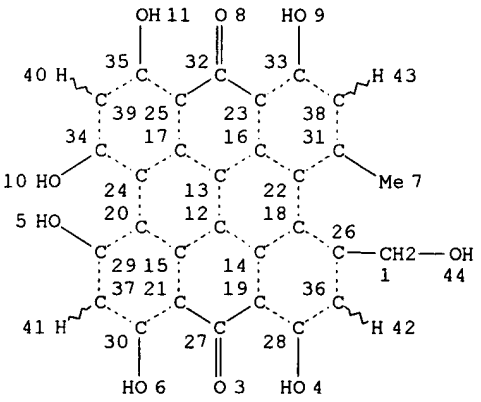


"C"

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE
L29 STR



"D"

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 43

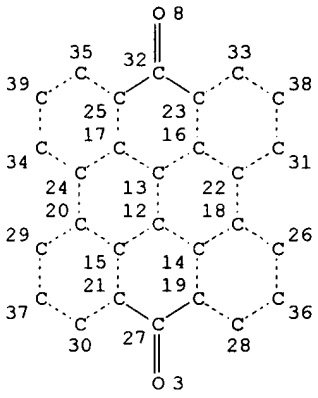
STEREO ATTRIBUTES: NONE
L31 36 SEA FILE=REGISTRY SUB=L24 SSS FUL (L26 OR L27 OR L28 OR L29)
L32 476 SEA FILE=HCAPLUS ABB=ON PLU=ON L31

I forgot to subtract out the subsets for the "E" & "F" provisos of Cl 18

=> d que 142

parent STR

L11 STR



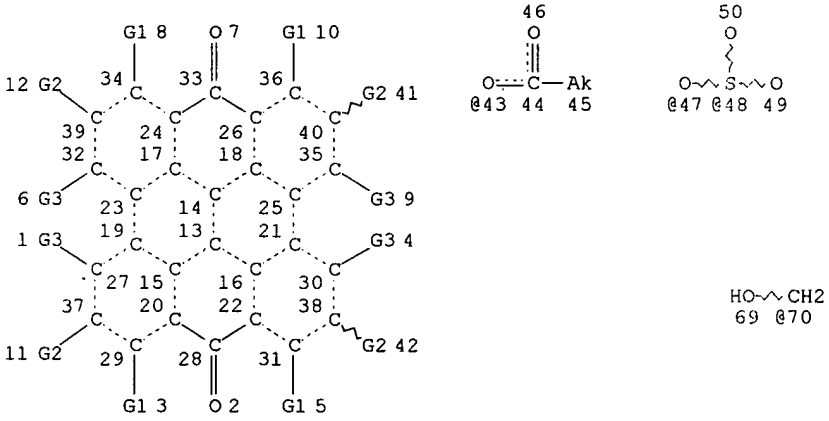
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

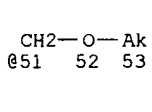
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

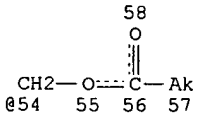
STEREO ATTRIBUTES: NONE
L13 183 SEA FILE=REGISTRY SSS FUL L11

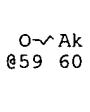
subset STR based on Cl 2

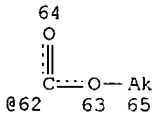
L22 STR



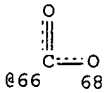








Page 1-A

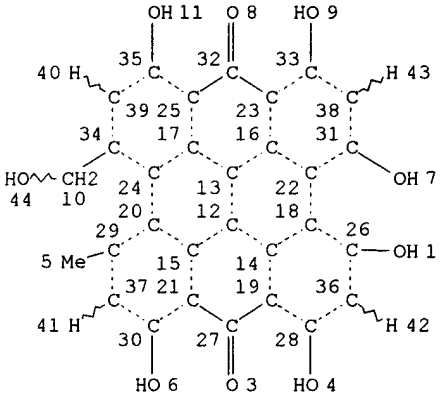


Page 2-A

VAR G1=H/OH/59/43
VAR G2=H/AK/X/47/48
VAR G3=H/AK/OH/59/43/70/51/54/62/66
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 68
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 69

STEREO ATTRIBUTES: NONE
L24 148 SEA FILE=REGISTRY SUB=L13 SSS FUL L22
L40 STR

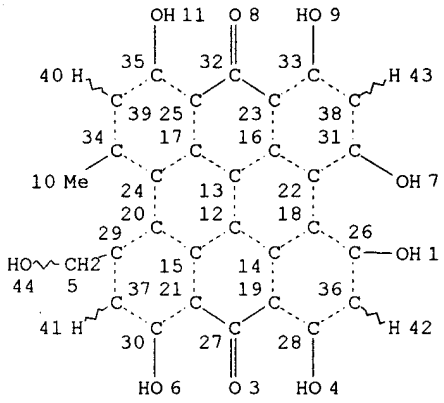


"E"

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE
L41 STR



"E"

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE
L42 1 SEA FILE=REGISTRY SUB=L24 SSS FUL L40 OR L41 only 1 cpd

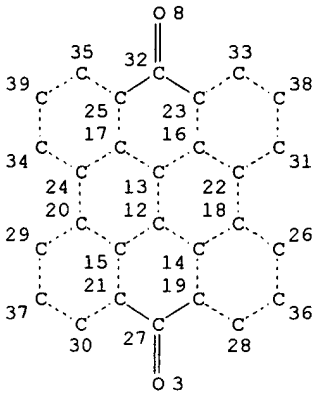
This display shows the cpds for cl 20 after subtracting out previously displayed cpds

=> d que 148

L6 12 SEA FILE=REGISTRY ABB=ON PLU=ON (548-04-9/BI OR 11079-53-1/BI OR 117-39-5/BI OR 143183-63-5/BI OR 153-18-4/BI OR 1617-53-4/BI OR 21637-25-2/BI OR 482-36-0/BI OR 52-39-1/BI OR 522-12-3/BI OR 55954-61-5/BI OR 9004-10-8/BI)

cpds from inventor search

L11 STR



parent STR

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

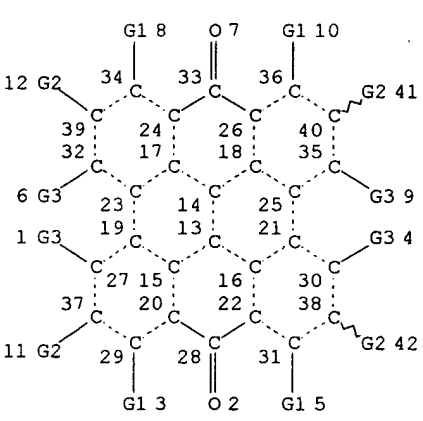
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

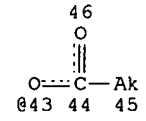
STEREO ATTRIBUTES: NONE

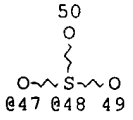
L13 183 SEA FILE=REGISTRY SSS FUL L11

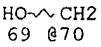
L22 STR

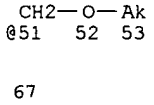
subset STR based on cl 2

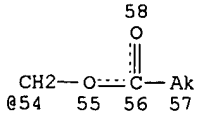


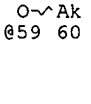


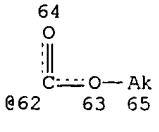




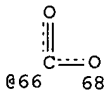








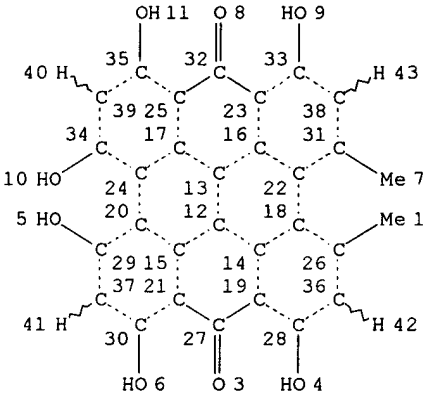
Page 1-A



Page 2-A
VAR G1=H/OH/59/43
VAR G2=H/AK/X/47/48
VAR G3=H/AK/OH/59/43/70/51/54/62/66
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 68
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 69

STEREO ATTRIBUTES: NONE
L24 148 SEA FILE=REGISTRY SUB=L13 SSS FUL L22
L26 STR

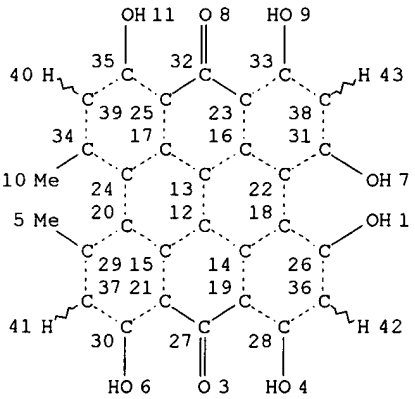


proviso cpd "A" of cl 18

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
L27 STR

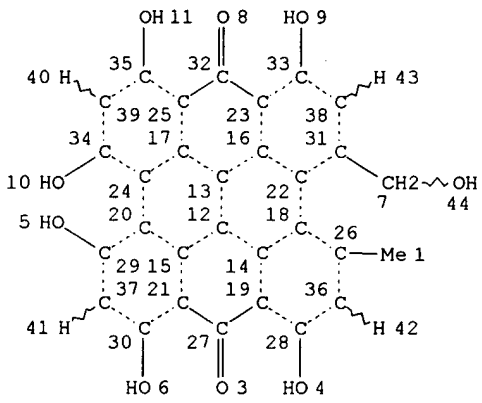


proviso "B" of cl 18

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
L28 STR

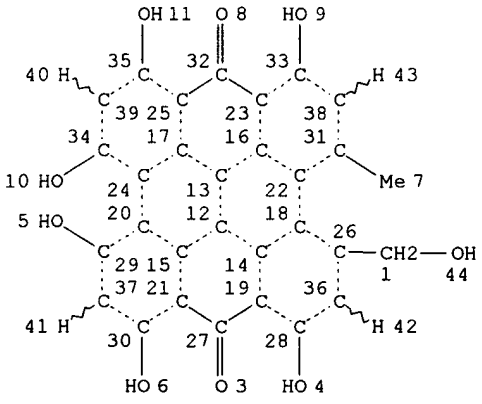


proviso "c" of cl 18

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE
L29 STR



proviso "d" of cl 18

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE
L31 36 SEA FILE=REGISTRY SUB=L24 SSS FUL (L26 OR L27 OR L28 OR L29)
L36 65 SEA FILE=REGISTRY ABB=ON PLU=ON (548-04-9/BI OR 120667-79-0/B

SEARCHED BY SUSAN HANLEY 305-4053

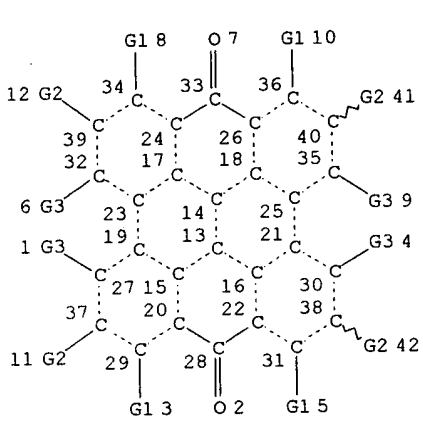
I OR 147593-87-1/BI OR 147593-89-3/BI OR 121263-19-2/BI OR 137363-72-5/BI OR 141436-78-4/BI OR 157301-83-2/BI OR 35082-49-6/BI OR 55954-61-5/BI OR 60483-14-9/BI OR 109-86-4/BI OR 111-77-3/BI OR 127180-29-4/BI OR 130942-84-6/BI OR 137632-06-5/BI OR 138674-26-7/BI OR 140208-17-9/BI OR 144700-81-2/BI OR 144788-48-7/BI OR 144941-32-2/BI OR 145987-20-8/BI OR 151765-07-0/BI OR 151765-17-2/BI OR 151766-28-8/BI OR 155092-33-4/BI OR 160919-80-2/BI OR 160919-81-3/BI OR 160919-82-4/BI OR 160919-83-5/BI OR 160919-84-6/BI OR 160919-85-7/BI OR 160919-86-8/BI OR 160919-87-9/BI OR 160919-88-0/BI OR 160919-89-1/BI OR 164397-05-1/BI OR 164397-06-2/BI OR 168323-98-6/BI OR 168323-99-7/BI OR 171782-05-1/BI OR 18521-72-7/BI OR 185672-52-0/BI OR 189113-18-6/BI OR 189113-21-1/BI OR 189113-23-3/BI OR 189113-25-5/BI OR 189113-27-7/BI OR 19267-89-1/BI OR 19697-87-1/BI OR 20516-32-9/BI OR 20752-80-1/BI OR 475-64-9/BI OR 481-70-9/BI OR 481-74-3/BI OR 518-82-1/BI OR 521-61-9/BI OR 52660-18-1/BI OR 55914-74-4/BI OR 602-06-2/BI OR 60935-17-3/BI OR 66-97-7/BI OR 79079-06-4/BI OR 88201-45-0/BI OR 9026-43-1/BI)

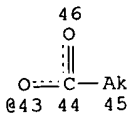
cpds already displayed

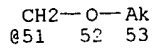
L37 75 SEA FILE=REGISTRY ABB=ON PLU=ON L6 OR L36

L44 STR

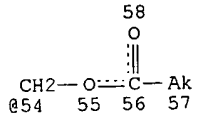
subset search for cpds of CL 20

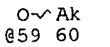


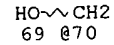




Ak @71







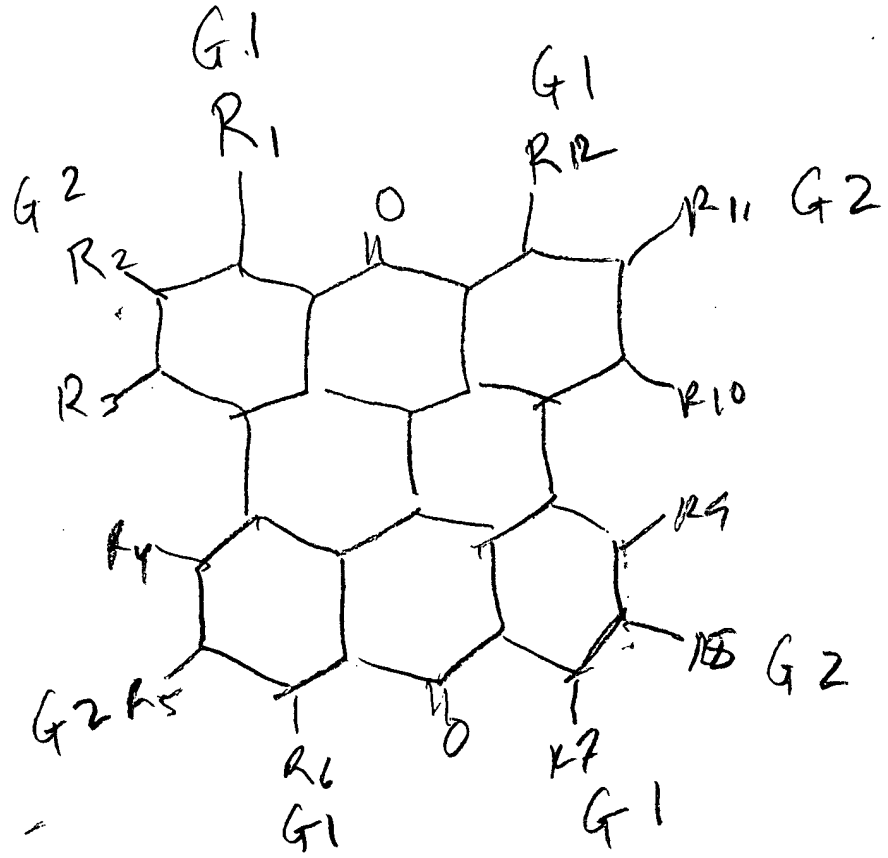
VAR G1=H/OH/59/43
VAR G2=H/71
VAR G3=H/71/OH/43/59/70/51/54
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC AT 45
GGCAT IS LOC AT 53
GGCAT IS LOC AT 57
GGCAT IS LOC AT 60
GGCAT IS LOC AT 71
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 59

STEREO ATTRIBUTES: NONE

L46 128 SEA FILE=REGISTRY SUB=L24 SSS FUL L44
L47 105 SEA FILE=REGISTRY ABB=ON PLU=ON L46 NOT L37
L48 77 SEA FILE=REGISTRY ABB=ON PLU=ON L47 NOT L31

77 cpds for CL 20



$G_1 = R_1 = R_7 = R_6 = R_{12}$ H / OH / OR / O-C(=O)-R

G_2 $R_2 = R_5 = R_8 = R_{11}$ H / AK / X / SO_3H

G_3 $R_3 = R_4 = R_9 = R_{10} =$

H / AK / OH / OR / O-C(=O)-R / CH_2OH / CH_2OR

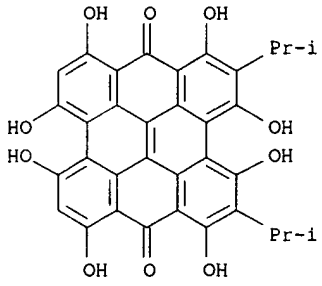
CH_2O-C(=O)-R -C(=O)-OH / R

L6 ANSWER 16 OF 16 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD
AN 1966-18731F [00] WPIDS
TI Rheumatism treatment.
DC B00
PA (TONE) TONERO A
CYC 1
PI BE 654914 A (196800)*
AB BE 654914 A UPAB: 19930831
Compns. containing as active agents extracts from ST. John's Wort (I) (**Hypericum perforatum**) and meadowsweet (II) (Filipendula
ulmaria) in ratios 20-60% and 40-80% respectively in the form of balms and ointments.
Treatment of rheumatism, **angina**, cardiac conditions, phlebitis, blood circulation conditions, psoriasis etc.
Compns. contng. 20-60% (I) and 40-80% (II) as under "Composition".
FS CPI
FA AB
MC CPI: B04-A07F; B12-A07; B12-D07; B12-D09; B12-E01; B12-F01; B12-F02

concern the structure of hypericin not really using it to treat the disorders in clm. 3, ie. hypertension.

=> d bib abs hitstr 154 1

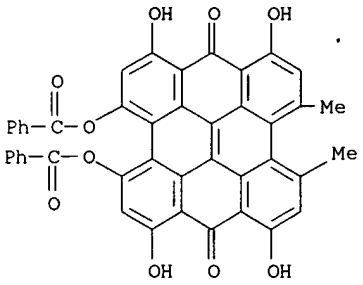
L54 ANSWER 1 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:762921 HCAPLUS
DN 132:78375
TI From the photosensitizer hypericin to the photoreceptor stentorin-the chemistry of phenanthroperylene quinones
AU Falk, Heinz
CS Institut fur Chemie der Johannes Kepler Universitat, Linz, A-4040, Austria
SO Angew. Chem., Int. Ed. (1999), 38(21), 3117-3136
CODEN: ACIEF5; ISSN: 1433-7851
PB Wiley-VCH Verlag GmbH
DT Journal; General Review
LA English
AB A review with 64 refs. on the chem. of phenanthroperylene quinones from the photosensitizer hypericin to the photoreceptor stentorin. The pursuit of the chem. of natural compds. contg. phenanthroperylene quinones substituted with hydroxyl and alkyl groups dates back nearly half a century. It experienced a renaissance within the last decade when it turned out that one of these compds., hypericin isolated from St. Johns wort-a phytotherapeutic drug known since antiquity-does not only exhibit ingestion deterrence, but also antiviral, photodynamically useful, and sedative properties. The fact that this group of phenanthroperylene quinones also contains the photosensory pigments of protozoa, such as stentorin, has addnl. contributed to this new interest in this class of compds. However, it is also the wealth of chem. and phys. problems that spurred the curiosity of scientists to probe the phenanthroperylene quinones in more detail. These problems are mainly a result of the network of tautomerism, dissocn., conformation, and assocn. equil. and the structural complexity thus caused by them. In keeping with the broad array of interdisciplinary investigations, which reach from synthetic org. chem. and spectroscopy to physiol. and medicine, this review will focus on a picture of the chem. aspects of this fascinating class of mols. framed by the background of its biol. aspects.
IT **147395-58-2**, Stentorin
RL: BOC (Biological occurrence); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PROC (Process)
(chem. aspects of phenanthroperylene quinones from the photosensitizer hypericin to the photoreceptor stentorin)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)



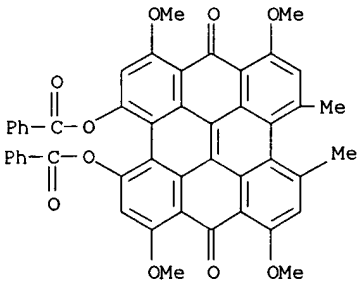
RE.CNT 278
RE
(1) Agostinis, P; Biochem Biophys Res Commun 1996, V220, P613 HCAPLUS
(2) Agostinis, P; Biochem Pharmacol 1995, V49, P1615 HCAPLUS
(3) Ahrer, W; Monatsh Chem 1998, V129, P643 HCAPLUS
(4) Ali Al-Akhras, M; J Photochem Photobiol B 1996, V34, P169 HCAPLUS
(5) Altmann, R; Monatsh Chem 1997, V128, P361 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr l54 2

L54 ANSWER 2 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:134526 HCAPLUS
DN 130:296542
TI Concerning regioselective photochemical intermolecular proton transfer from hypericin
AU Obermueller, Roland A.; Schuetz, Gerhard J.; Gruber, Hermann J.; Falk, Heinz
CS Inst. Chem., Johannes Kepler Univ., Linz, A-4040, Austria
SO Monatsh. Chem. (1999), 130(2), 275-281
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer-Verlag Wien
DT Journal
LA English
AB Using epifluorescence microscopy on lipid vesicles contg. hypericin or several of its O-alkylated derivs. together with a fluorescence pH indicator, it was shown that upon excitation of the resp. hypericinate ion an excited-state-derived proton is transferred to the indicator mol. In addn., it could also be unequivocally derived that this proton originates from one of the peri-hydroxyl groups of the pigment.
IT **223115-06-8 223115-11-5**
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process)
(regioselective photochem. intermol. proton transfer from hypericin)
RN 223115-06-8 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis(benzoyloxy)-1,6,8,13-tetrahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)



RN 223115-11-5 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis(benzoyloxy)-1,6,8,13-tetramethoxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

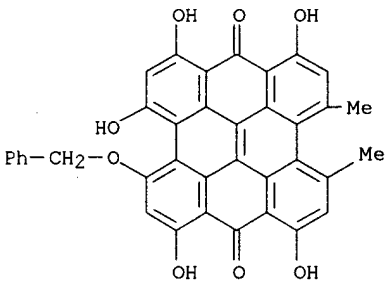


RE.CNT 31
RE
(1) Agostinis, P; Biochem Biophys Res Commun 1996, V220, P613 HCAPLUS
(2) Altmann, R; Monatsh Chem 1997, V128, P571 HCAPLUS
(3) Amer, A; Monatsh Chem 1998, V129, P1237 HCAPLUS

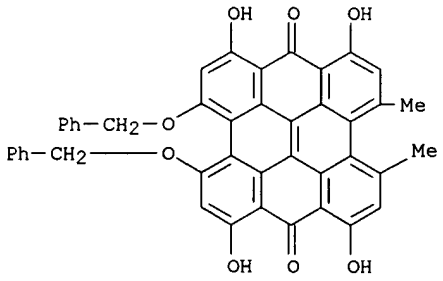
(4) Babcock, G; Biochemistry, 1989, V28, P9557 HCAPLUS
(5) Carpenter, S; Photochem Photobiol 1991, V53, P169 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr l54 3

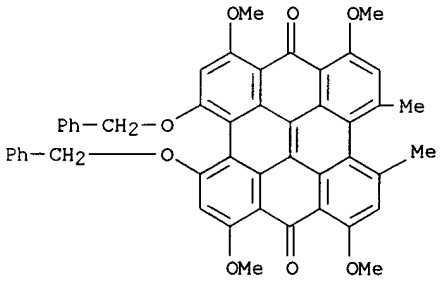
L54 ANSWER 3 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:23725 HCAPLUS
DN 130:95421
TI The dissociation and tautomerization equilibria of hypericin. Alkyl-protected hydroxyl derivatives
AU Amer, Atef M.; Falk, Heinz; Tran, Huyen T. N.
CS Institut Chemie, Johannes Kepler Universitaet, Linz, A-4040, Austria
SO Monatsh. Chem. (1998), 129(12), 1237-1244
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer-Verlag Wien
DT Journal
LA English
AB 3-Benzyl-, 3,4-dibenzyl-, 3,4-dibenzyl-1,6,8,13-tetramethyl-, and 1,6,8,13-tetramethylhypericin were synthesized by alkylation and dealkylation procedures starting from hypericin. The pKa value correlation of these derivs. allowed the unequivocal assignment of the protonation and deprotonation pKa values of hypericin. Thus, for hypericin the pKa of .apprxeq.-6 was assigned to the C:O groups, that of .apprxeq.2 to the deprotonation of 1 OH group in the bay-positions 3/4, and that of .apprxeq.9 was found to be characteristic of the bay-peri-diphenolate ion. None of the changes in the spectra characteristic of changes in the tautomeric equil. could be found for these derivs. Thus, it was concluded that the undisturbed peripheral OH groups of hypericin have to be present to allow for tautomeric changes.
IT **219547-31-6P 219547-32-7P 219547-33-8P 219547-34-9P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(prepn. and deprotonation and tautomerization equil. of alkyl-protected hydroxyl derivs. of hypericin)
RN 219547-31-6 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,6,8,13-pentahydroxy-10,11-dimethyl-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



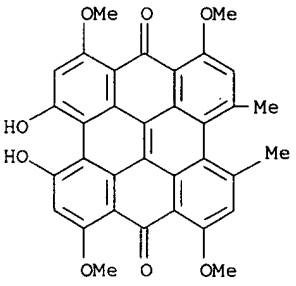
RN 219547-32-7 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,13-tetrahydroxy-3,4-dimethyl-10,11-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)



RN 219547-33-8 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,13-tetramethoxy-3,4-dimethyl-10,11-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)



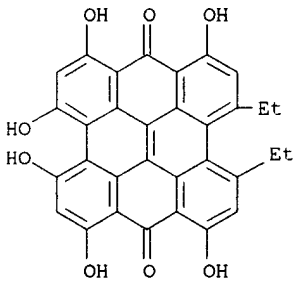
RN 219547-34-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-dihydroxy-1,6,8,13-tetramethoxy-10,11-dimethyl- (9CI) (CA INDEX NAME)



RE.CNT 30
RE
(1) Agostinis, P; Biochem Biophys Res Commun 1996, V220, P613 HCAPLUS
(2) Ahrer, W; Monatsh Chem 1998, V129, P643 HCAPLUS
(3) Altmann, R; Monatsh Chem 1997, V128, P571 HCAPLUS
(4) Carpenter, S; Photochem Photobiol 1991, V53, P169 HCAPLUS
(6) Etzlstorfer, C; Monatsh Chem 1993, V124, P923 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

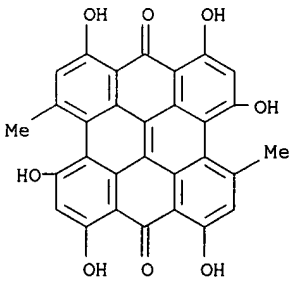
=> d bib abs hitstr l54 4

L54 ANSWER 4 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:432997 HCAPLUS
DN 129:244909
TI Studies on synthesis and anti-HIV activity of hypericin and ethylhypericin
AU Zhao, Jin; Zhang, Zhiping; Chen, Hongshan; Chen, Xianghong
CS Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences, Beijing, 100050, Peop. Rep. China
SO Yaoxue Xuebao (1998), 33(1), 67-71
CODEN: YHHPAL; ISSN: 0513-4870
PB Chinese Academy of Medical Sciences, Institute of Materia Media
DT Journal
LA Chinese
AB Condensed polycyclic anthraquinone hypericin and its analogs showed antiretrovirus activities, including human immunodeficiency virus (HIV). Activity of Ethylhypericin synthesized from butanone was compared with hypericin. The ethylhypericin was slightly more effective than hypericin in HIV retrotranscription test.
IT **213138-46-6P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and anti-HIV activity of hypericin and ethylhypericin)
RN 213138-46-6 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-diethyl-1,6,8,10,11,13-hexahydroxy- (9CI) (CA INDEX NAME)



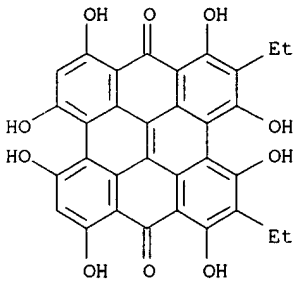
=> d bib abs hitstr l54 5

L54 ANSWER 5 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:399546 HCAPLUS
DN 129:202778
TI Quantum chemistry calculation study on photosensitization of perylenequinonoid derivatives
AU Zhang, Hong-Yu
CS Dep. Biology, Shandong Normal Univ., Jinan, 250014, Peop. Rep. China
SO Shengwu Huaxue Yu Shengwu Wuli Xuebao (1998), 30(3), 272-276
CODEN: SHWPAU; ISSN: 0582-9879
PB Shanghai Kexue Jishu Chubanshe
DT Journal
LA Chinese
AB AM1 method has been employed to calc. perylenequinonoid photosensitizers (PQDs). Parameters such as heat of formation (HF), HOMO, LUMO levels and spin d. distribution of free radicals are obtained. In combination with exptl. results, several photophys. and photochem. characteristics of PQDs are elucidated, which lay a foundation for investigating photosensitive mechanisms of PQDs further.
IT **41689-58-1**, Isohypericin
RL: PRP (Properties)
(quantum chem. calcn. study on photosensitization of perylenequinonoid derivs.)
RN 41689-58-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,6,8,10,13-hexahydroxy-4,11-dimethyl- (9CI) (CA INDEX NAME)

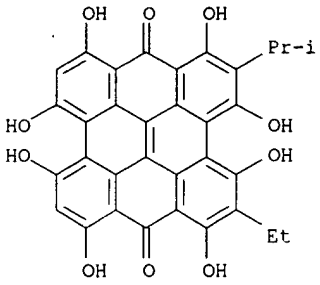


=> d bib abs hitstr l54 6

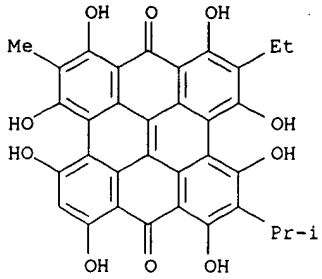
L54 ANSWER 6 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:348082 HCAPLUS
DN 129:95350
TI On the structure of oxyblepharismin and its formation from blepharismin
AU Spitzner, Dietrich; Hofle, Gerhard; Klein, Iris; Pohlan, Silke; Ammermann, Dieter; Jaenicke, Lothar
CS Institut fur Chemie, Universitat Hohenheim, Stuttgart, D-70599, Germany
SO Tetrahedron Lett. (1998), 39(23), 4003-4006
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
AB The blepharismins from Blepharisma japonicum give the corresponding oxyblepharismins on irradn. in vitro and in vivo. The chem. structures of these compds. are elucidated and a mechanism is given for this unusual transformation.
IT **209669-10-3P**, Stentorin A **209669-11-4P**, Stentorin B
209669-31-8P, Stentorin D **209669-32-9P**, Stentorin E
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure of oxyblepharismin and formation from blepharismin)
RN 209669-10-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-diethyl-1,3,4,6,8,10,11,13-octahydroxy- (9CI) (CA INDEX NAME)



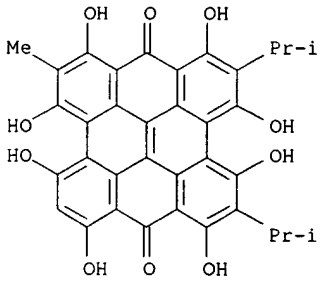
RN 209669-11-4 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2-ethyl-1,3,4,6,8,10,11,13-octahydroxy-5-(1-methylethyl)- (9CI) (CA INDEX NAME)



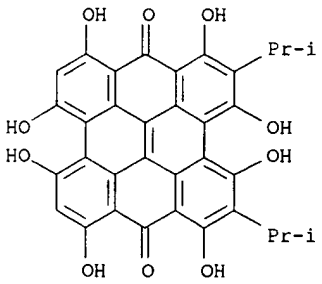
RN 209669-31-8 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 5-ethyl-1,3,4,6,8,10,11,13-octahydroxy-9-methyl-2-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 209669-32-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-9-methyl-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

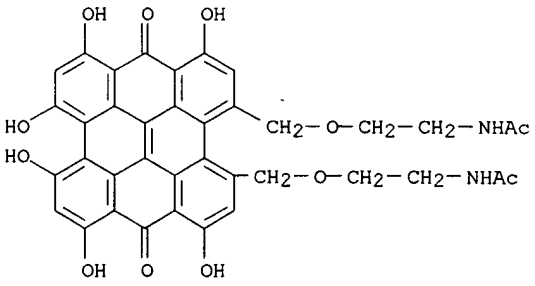


IT **147395-58-2P**, Stentorin C
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure of oxyblepharismin and formation from blepharismin)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

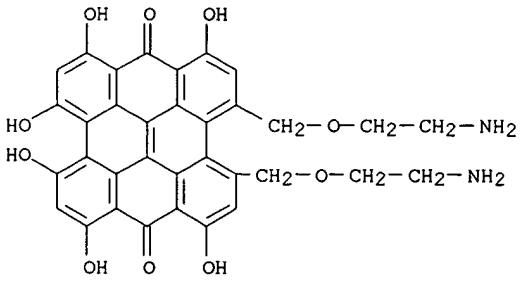


=> d bib abs hitstr 154 7

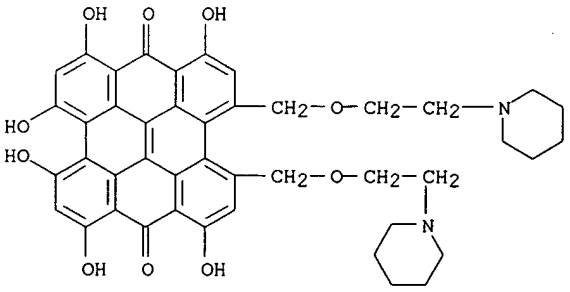
L54 ANSWER 7 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:190509 HCAPLUS
DN 128:257278
TI Synthesis and properties of hypericins substituted with acidic and basic residues. Hypericintetrasulfonic acid. A water soluble hypericin derivative
AU Falk, Heinz; Sarhan, Abd-El-Wareth A. O.; Tran, Huyen T. N.; Altmann, Robert
CS Inst. Chemie, Johannes Kepler Univ., Linz, A-4040, Austria
SO Monatsh. Chem. (1998), 129(3), 309-318
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer-Verlag Wien
DT Journal
LA English
AB Sulfonation of hypericin leads to the corresponding di-, tri-, and tetrasulfonates. The latter is water-sol. up to millimolar solns. Homoaggregate formation (J-aggregates) was obsd. only >5.cntdot.10-4 mol/l. In aq. soln., the hypericintetrasulfonate exists as its bay-phenolate with most of the sulfonates dissocd. Thus, a water-sol. hypericin deriv., which in contrast to hypericin is not prone to homoassocn., is presented. Hypericintetrasulfonate forms heteroassocs. with serum albumin, DNA, and .gamma.-cyclodextrin. Hypericin derivs. with primary and tertiary amino group appendages at the hypericin Me groups were synthesized. However, upon salt formation or quaternization these derivs. became virtually insol. in all common solvents including water.
IT **205384-03-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of hypericinsulfonates and amino hypericins)
RN 205384-03-8 HCAPLUS
CN Acetamide, N,N'-[(7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxophenanthro[1,10,9,8-opqra]perylene-3,4-diyl)bis(methyleneoxy-2,1-ethanediyl)]bis- (9CI) (CA INDEX NAME)



IT **205384-04-9P 205384-07-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of hypericinsulfonates and amino hypericins)
RN 205384-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis[(2-aminoethoxy)methyl]-1,6,8,10,11,13-hexahydroxy- (9CI) (CA INDEX NAME)

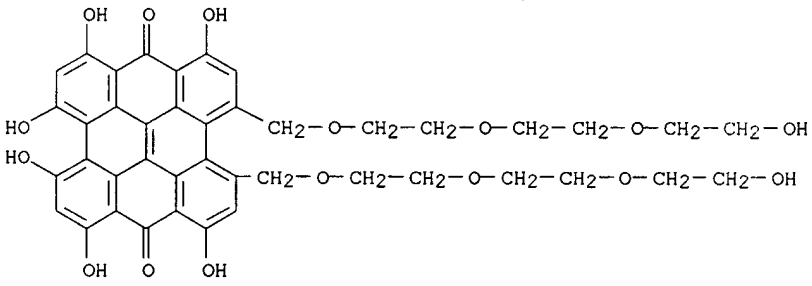


RN 205384-07-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[2-(1-piperidinyl)ethoxy]methyl]- (9CI) (CA INDEX NAME)



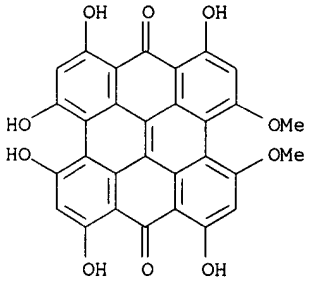
=> d bib abs hitstr l54 8

L54 ANSWER 8 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:190503 HCAPLUS
DN 128:257277
TI Synthesis and properties of ionophore conjugated hypericin derivatives
AU Altmann, Robert; Falk, Heinz; Gruber, Hermann J.
CS Inst. Chemie, Johannes Kepler Univ., Linz, A-4040, Austria
SO Monatsh. Chem. (1998), 129(3), 235-244
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer-Verlag Wien
DT Journal
LA English
AB Two types of derivs. substituted with ionophoric residues at the .omega.,.omega.'-Me groups of hypericin were synthesized. On the one hand, an open-chain triethylene glycol deriv. did not form stable complexes with alkali metal ions. Embedded as its detergent salt in lipid bilayer membranes it did not provide specific H+, Na+, or K+ channels. On the other hand, crown-4 and crown-5 hypericin derivs. were able to complex Na+ and K+ ions, with the crown-5 compd. forming a stable K crown complex. In such systems, the hypericinate ion is intramolecularly compensated by the complexed cation, thereby forming an extremal structure within the series of hypericinates.
IT **171782-06-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and properties of ionophore conjugated hypericin derivs.)
RN 171782-06-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]methyl]- (9CI) (CA INDEX NAME)

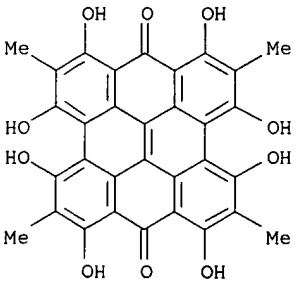


=> d bib abs hitstr l54 9

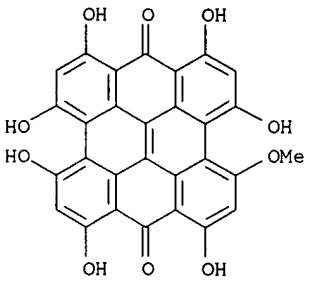
L54 ANSWER 9 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:74125 HCAPLUS
DN 128:140417
TI Hypericin, hypocrellin, and model compounds: steady-state and time-resolved fluorescence anisotropies
AU Das, K.; Dertz, E.; Paterson, J.; Zhang, W.; Kraus, G. A.; Petrich, J. W.
CS Department of Chemistry, Iowa State University, Ames, IA, 50011-3111, USA
SO J. Phys. Chem. B (1998), 102(8), 1479-1484
CODEN: JPCBFK; ISSN: 1089-5647
PB American Chemical Society
DT Journal
LA English
AB Steady-state and time-resolved fluorescence anisotropies of hypericin (I), hypocrellin (II), and 5 other analogs were measured. The steady-state excitation anisotropies for each of these compds. has a broad min. at .apprx.400 nm with a neg. value. At the blue and red edges of the spectrum the value of the anisotropy is pos. Time-resolved fluorescence-anisotropy measurements were performed for both I and II at excitation wavelengths of 300 and 570 nm. The limiting anisotropies are in excellent agreement with the corresponding steady-state values. These results are discussed in terms of the directions of the transition dipoles connecting the ground state to various excited states. The role of conformational isomers and tautomers in the ground and excited states is also considered.
IT **172226-96-9P 172226-97-0P 172226-98-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(steady-state and time-resolved fluorescence anisotropies of hypericin, hypocrellin and model compds.)
RN 172226-96-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy- (9CI) (CA INDEX NAME)



RN 172226-97-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5,9,12-tetramethyl- (9CI) (CA INDEX NAME)

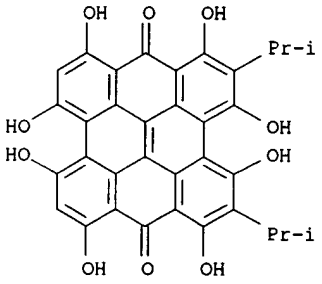


RN 172226-98-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,13-heptahydroxy-11-methoxy- (9CI) (CA INDEX NAME)



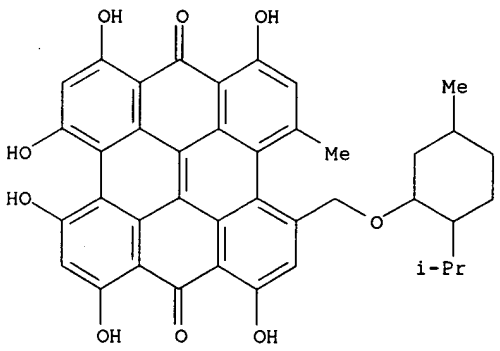
=> d bib abs hitstr l54 10

L54 ANSWER 10 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:704005 HCAPLUS
DN 128:11224
TI Light and phosphorylation-induced conformational change in phytochrome a and photoinduced electron transfer from stentorin
AU Wells, Todd Alan
CS Univ. of Nebraska, Lincoln, NE, USA
SO (1997) 123 pp. Avail.: UMI, Order No. DA9736958
From: Diss. Abstr. Int., B 1997, 58(6), 3027
DT Dissertation
LA English
AB Unavailable
IT **147395-58-2**, Stentorin
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(light and phosphorylation-induced conformational change in phytochrome a and photoinduced electron transfer from stentorin)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

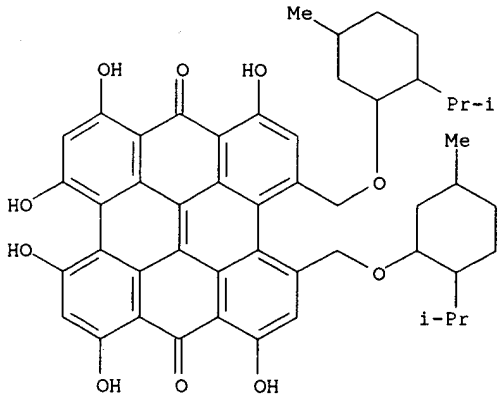


=> d bib abs hitstr l54 11

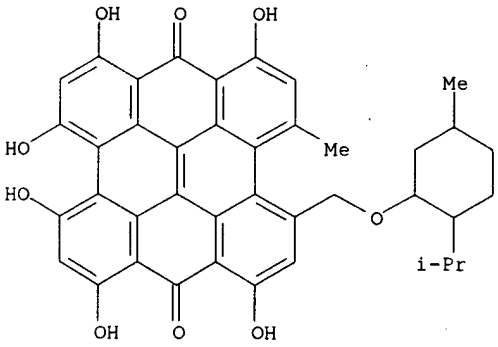
L54 ANSWER 11 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:619494 HCAPLUS
DN 127:307250
TI Chiroptical properties and absolute configurations of the hypericin chromophore propeller enantiomers
AU Altmann, R.; Etzlstorfer, C.; Falk, H.
CS Institut Chemie, Johannes Kepler Universitat, Linz, A-4040, Austria
SO Monatsh. Chem. (1997), 128(8/9), 785-793
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer
DT Journal
LA English
AB The diastereomeric mono- and bis-.omega.-appended (R)-menthyl hypericins were studied by absorption spectroscopy, CD measurements, application of the C2 rule, and semiempirical calcns. The abs. configuration (P) is assigned to the inherently chiral phenanthroperylene quinone chromophore of hypericin, the bay-hypericinate ion, and the 1,6-dioxo tautomer displaying a neg. Cotton effect of their long wavelength absorption band. From these results and according to the pos. chiroptical sign of their long wavelength bands, the abs. configuration (M) could be assigned to the stentorin chromophore in the native pigments.
IT **197156-50-6 197156-51-7 197251-98-2**
197251-99-3
RL: PRP (Properties)
(chiroptical properties and abs. configuration of menthyl hypericins)
RN 197156-50-6 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-methyl-11-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)



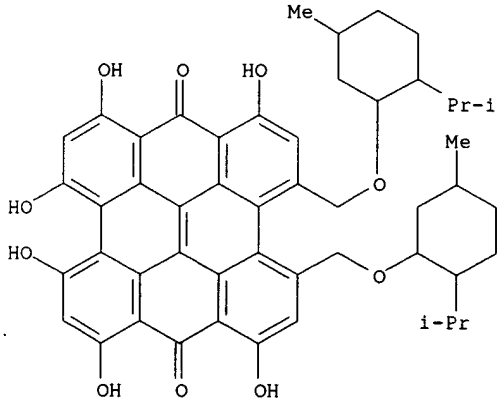
RN 197156-51-7 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)



RN 197251-98-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-methyl-11-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)

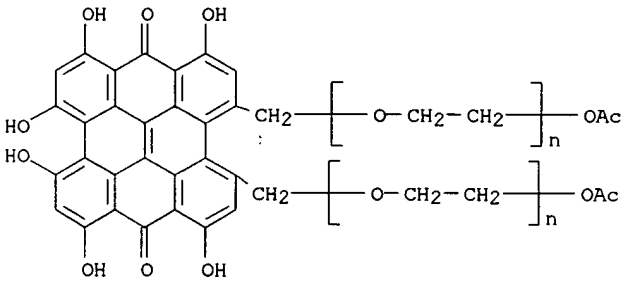


RN 197251-99-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)



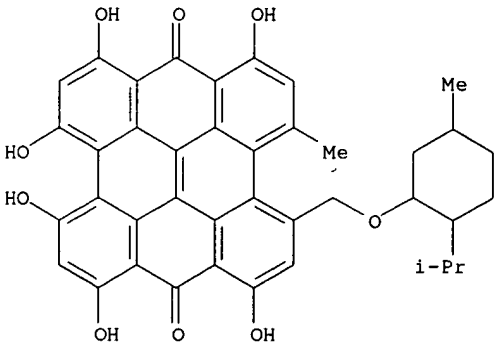
=> d bib abs hitstr l54 12

L54 ANSWER 12 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:619470 HCAPLUS
DN 127:293065
TI The deprotonation and protonation equilibria of a hypericin derivative in aqueous solution
AU Altmann, R.; Falk, H.
CS Institut Chemie, Johannes Kepler Universitat, Linz, A-4040, Austria
SO Monatsh. Chem. (1997), 128(6/7), 571-583
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer
DT Journal
LA English
AB A hypericin deriv. .omega.,.omega.'-appended at the Me groups with 2 polyethylene glycol moieties (.apprx.23 units long) and capped with acetyl groups was synthesized starting from emodin. This deriv. proved to water-sol. and was investigated by spectrophotometric titrn. and electrophoresis. Deprotonation at the bay-region OH group was obsd. at pKa = 1.6. This was followed by a 2nd deprotonation step of a peri-OH group at pKa = 9.4. This deriv. could be protonated at the CO group at pKa = -5.7. From pKa detns. in H2O/EtOH mixts. the corresponding pKa values of hypericin itself were extrapolated to the aq. phase. This resulted in estd. pKa values of 1.8, 9.2, and -6.0, resp.
IT **197228-68-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(deprotonation and protonation equil. of hypericin deriv. in aq. soln.)
RN 197228-68-5 HCAPLUS
CN Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[(7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxophenanthro[1,10,9,8-opqra]perylene-3,4-diyl)bis(methylene)]bis[.omega.-(acetyloxy)- (9CI) (CA INDEX NAME)

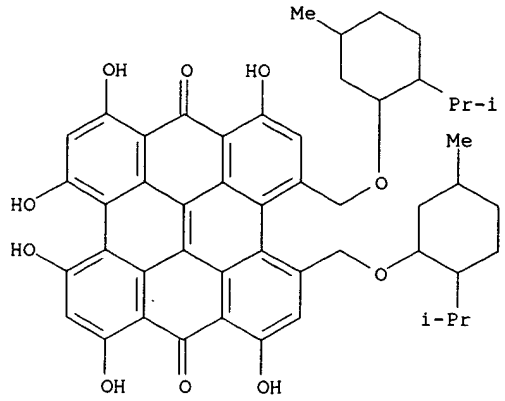


=> d bib abs hitstr 154 13

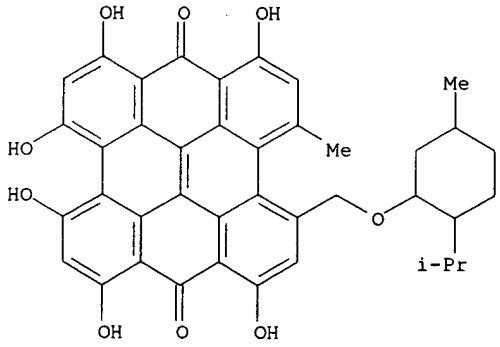
L54 ANSWER 13 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:611643 HCAPLUS
DN 127:307249
TI Concerning the enantiomerization barrier of hypericin
AU Altmann, R.; Etzlstorfer, C.; Falk, H.
CS Institut Chemie, Johannes Kepler Universitat, Linz, A-4040, Austria
SO Monatsh. Chem. (1997), 128(4), 361-370
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer
DT Journal
LA English
AB The syntheses of .omega.-(R)-menthyl and .omega.,.omega.'-bis-(R)-menthyl derivs. of hypericin were achieved, and the corresponding diastereomers could be sepd. The equil. between the resp. diastereomers are slightly displaced in favor of the chromatog. faster moving ones. Kinetic measurements on these easily equilibrating diastereomers provided an Arrhenius activation energy for the interconversion barrier between the 2 propeller conformers of 83 and 89 kJ/mol. The .omega.-menthyl residues are of minor relevance to the height of this barrier, as is also the case for the bay hydroxyl ionization and quinone tautomerization equil. It was thus concluded that the intrinsic barrier for the propeller conformer enantiomerization of hypericin is in the order of 80 kJ/mol. These results are in accord with those obtained from semiempirical calcns.
IT **197156-50-6P 197156-51-7P 197251-98-2P**
197251-99-3P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., enantiomerization, and kinetics thereof of hypericin menthyl derivs.)
RN 197156-50-6 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-methyl-11-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)



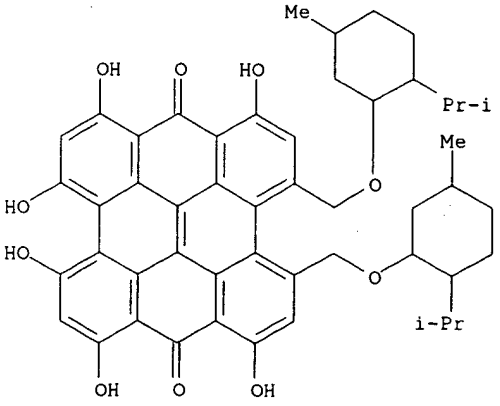
RN 197156-51-7 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)



RN 197251-98-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-methyl-11-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)

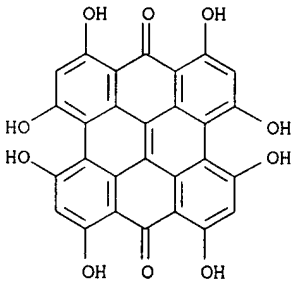


RN 197251-99-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)



=> d bib abs hitstr l54 14

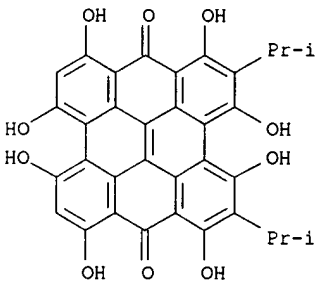
L54 ANSWER 14 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:611642 HCAPLUS
DN 127:278101
TI Concerning bay salt and peri chelate formation of hydroxyphenanthroperylene quinones (fringelites)
AU Falk, H.; Mayr, E.
CS Institut Chemie, Johannes Kepler Universitat, Linz, A-4040, Austria
SO Monatsh. Chem. (1997), 128(4), 353-360
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer
DT Journal
LA English
AB The bathochromic shifts in the diffuse reflectance UV/Vis spectra of certain fringelite-contg. fossil species and the exceptional chem. stability of the fringelites and their resistance against leaching on a geol. time scale can be understood from the unique complexation behavior of fringelites with transition metal ions. According to an absorption spectroscopic study of the model system fringelite D-alk. earth metal and transition metal ions, fringelites are able to form peri chelate complexes. In addn., fringelites bearing bay hydroxyl groups are able to form polymeric phenolates with transition metal ions as well as with alk. earth metal ions. This behavior leads to a complex network lattice consisting of these polymeric chains crosslinked via chelate coordination of the peri regions to transition metal ions like Fe.
IT **196873-95-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(salt formation and chelation of fringelite)
RN 196873-95-7 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-, calcium salt (1:1) (9CI) (CA INDEX NAME)



● Ca

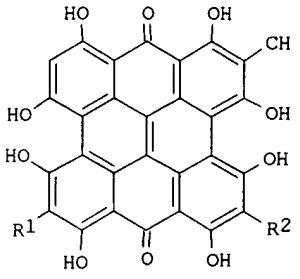
=> d bib abs hitstr l54 15

L54 ANSWER 15 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:590902 HCAPLUS
DN 127:270322
TI Electron Transfer Quenching and Photoinduced EPR of Hypericin and the Ciliate Photoreceptor Stentorin. [Erratum to document cited in CA126:137514]
AU Wells, Todd A.; Losi, Aba; Dai, Renke; Scott, Paul; Anderson, Michael; Redepenning, Jody; Park, Su-Moon; Golbeck, John; Song, Pill-Soon
CS Departments of Chemistry and Biochemistry, University of Nebraska, Lincoln, NE, 68588-0304, USA
SO J. Phys. Chem. A (1997), 101(40), 7460
CODEN: JPCAFH; ISSN: 1089-5639
PB American Chemical Society
DT Journal
LA English
AB Page 366. The names of Michael Anderson and Jody Redepenning have been added to the list of authors.
IT **147395-58-2**, Stentorin
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process)
(photoinduced electron-transfer quenching of hypericin and stentorin excited singlet states (Erratum))
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)



=> d bib abs hitstr 154 16

L54 ANSWER 16 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:452084 HCAPLUS
DN 127:108798
TI Synthesis of stentorin
AU Cameron, Donald W.; Riches, Andrew G.
CS School of Chemistry, The University of Melbourne, Parkville, VIC. 3052, Australia
SO Aust. J. Chem. (1997), 50(4), 409-424
CODEN: AJCHAS; ISSN: 0004-9425
PB CSIRO
DT Journal
LA English
GI

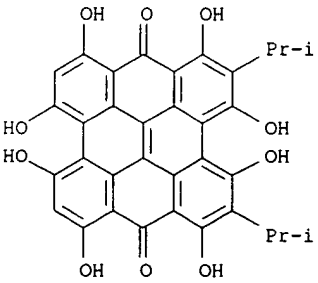


I

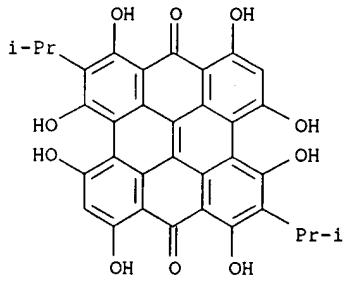
AB The two isomeric structures I (R1 = H, R2 = CHMe2) and I (R1 = CHMe2, R2 = H) proposed for the photodynamic pigment stentorin were both synthesized for the first time, thereby allowing unambiguous identification of the natural material as I (R1 = H, R2 = CHMe2). Synthesis of these highly condensed arom. systems involved controlled oxidative couplings of the new anthrones II (R3 = CHMe2, R4 = H; R3 = H, R4 = CHMe2), each synthesized by regiocontrolled cycloaddn.

IT **147395-58-2P**, Stentorin **192379-26-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(mol. structure of stentorin via regiocontrolled synthesis)

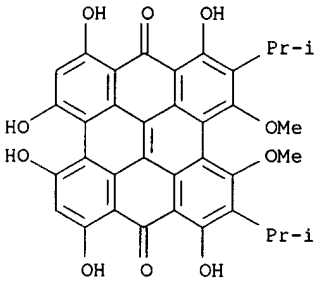
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)



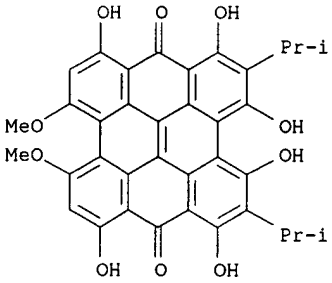
RN 192379-26-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,9-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



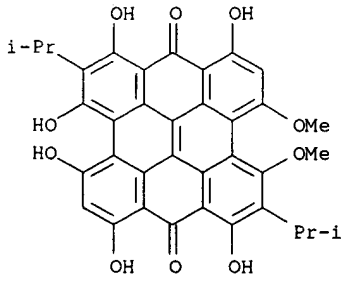
IT **162975-31-7P 162975-32-8P 162975-33-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(mol. structure of stentorin via regiocontrolled synthesis)
RN 162975-31-7 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,10,11,13-hexahydroxy-3,4-dimethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 162975-32-8 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

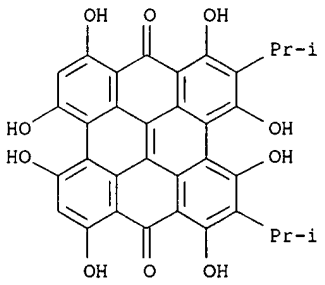


RN 162975-33-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-2,9-bis(1-methylethyl)- (9CI) (CA INDEX NAME)


OH
O
OH
i-Pr
HO
OMe
HO
OMe
Pr-i
OH
O
OH

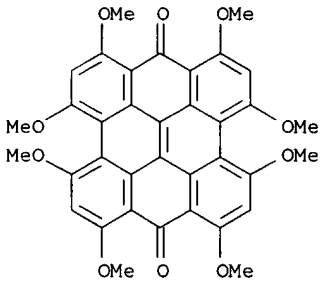
=> d bib abs hitstr 154 17

L54 ANSWER 17 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:266863 HCAPLUS
DN 126:263812
TI Concerning the acidity and hydrogen bonding of hydroxyphenanthroperylene quinones like fringelite D, hypericin, and stentorin
AU Etzlstorfer, C.; Falk, H.; Mayr, E.; Schwarzinger, S.
CS Institut Chemie, Johannes Kepler Univ., Linz, A-4040, Austria
SO Monatsh. Chem. (1996), 127(12), 1229-1237
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer
DT Journal
LA English
AB The strongly enhanced acidity of the bay OH group as compared to the resp. peri OH groups of fringelite D, hypericin, and stentorin could be rationalized on the basis of a vinylogous carboxylate and was nicely corroborated by semiempirical calcns. of the AM1 type. Exptl. data obtained from several independent exptl. methods, like polarized absorption spectroscopy, hole burning, and isotope effects, as well as from semiempirical AM1 and 6-31G level ab initio calcns. conclusively pointed to dissym. H bonding systems in both the peri and bay regions of the corresponding bay phenolate ions.
IT **147395-58-2**, Stentorin
RL: PRP (Properties)
(acidity and hydrogen bonding of hydroxyphenanthroperylene quinones)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)



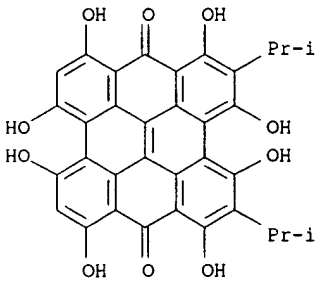
=> d bib abs hitstr l54 18

L54 ANSWER 18 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:224048 HCAPLUS
DN 126:299578
TI Excited-State Photophysics of Hypericin and Its Hexamethoxy Analog: Intramolecular Proton Transfer as a Nonradiative Process in Hypericin
AU English, D. S.; Zhang, W.; Kraus, G. A.; Petrich, J. W.
CS Department of Chemistry, Iowa State University, Ames, IA, 50011, USA
SO J. Am. Chem. Soc. (1997), 119(13), 2980-2986
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB The excited-state photophysics of the light induced antiviral agent, hypericin, are compared with those of its methylated analog, hexamethoxyhypericin. This comparison is instructive in understanding both the ground- and the excited-state properties of hypericin. That the hexamethoxy analog has no labile protons that can be transferred, that it cannot protonate its own carbonyl groups, that it has a reduced fluorescence quantum yield and lifetime with respect to hypericin, and that it exhibits no stimulated emission or, more specifically, rise time in stimulated emission completely support our emerging model of the hypericin photophysics. The results are consistent with the presence of intramol. excited-state proton transfer in hypericin but not in its methylated analog.
IT **168287-28-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(in prepn. of hexamethoxyhypericin)
RN 168287-28-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octamethoxy- (9CI) (CA INDEX NAME)



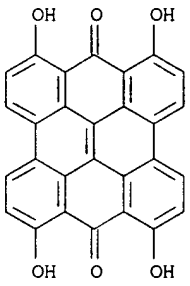
=> d bib abs hitstr l54 19

L54 ANSWER 19 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:140636 HCAPLUS
DN 126:137514
TI Electron Transfer Quenching and Photoinduced EPR of Hypericin and the Ciliate Photoreceptor Stentorin
AU Wells, Todd A.; Losi, Aba; Dai, Renke; Scott, Paul; Park, Su-Moon; Golbeck, John; Song, Pill-Soon
CS Departments of Chemistry and Biochemistry, University of Nebraska, Lincoln, NE, 68588-0304, USA
SO J. Phys. Chem. A (1997), 101(4), 366-372
CODEN: JPCAFH; ISSN: 1089-5639
PB American Chemical Society
DT Journal
LA English
AB Time-correlated single photon counting was used to observe dynamic quenching of the hypericin and stentorin excited singlet states. The fluorescence quenching data for hypericin and stentorin were interpreted in terms of electron transfer. The obsd. correlation between free energy change of electron transfer and quenching rate const. suggests that quenching proceeds via electron transfer from hypericin and stentorin to the quenchers. EPR spectra for hypericin, stentorin, and stentorin chromoprotein demonstrated that free radical formation was initiated or enhanced by visible light and that similar radical species were produced in each sample. Furthermore, the EPR signal for stentorin was significantly enhanced by 1,4-benzoquinone, but the overall shape and g-value was unchanged. We suggest that electron transfer in the excited state of these chromophores results in the formation of a cation radical. This electron transfer is a rapid and efficient pathway for deactivation of hypericin and stentorin excited singlet states and should be considered when discussing the photoreactivity of hypericin as a photodynamic agent and of stentorin as the Stentor coeruleus photoreceptor.
IT **147395-58-2**, Stentorin
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process)
(photoinduced electron-transfer quenching of hypericin and stentorin excited singlet states)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

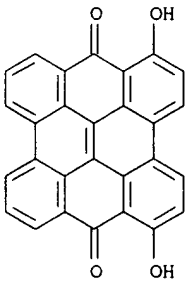


=> d bib abs hitstr l54 20

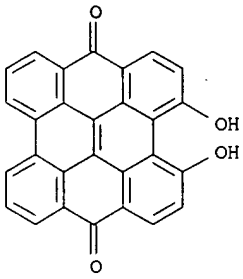
L54 ANSWER 20 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:684927 HCAPLUS
DN 126:74439
TI Structural aspects and electronic absorption of the hydroxyphenanthroperylene quinones fringelite D, hypericin, and stentorin
AU Etzlstorfer, C.; Falk, H.; Mueller, N.; Tran, T. N. H.
CS Inst. Chem., Johannes Kepler Univ. Linz, Linz, A-4040, Austria
SO Monatsh. Chem. (1996), 127(6/7), 659-668
CODEN: MOCMB7; ISSN: 0026-9247
PB Springer
DT Journal
LA English
AB PPP semiempirical quantum chem. calcns. of absorption spectra were performed for hypericin, fringelite D, stentorin, and their resp. conformers, tautomers, and deprotonated species. The results agree with the exptl. absorption spectra of hypericin, fringelite D, and stentorin, their deprotonated species, and the polarized absorption spectra of an .omega.,.omega.'-long chain appended hypericin deriv. embedded in stretched polyethylene.
IT **122194-30-3 141600-17-1 141600-18-2 147395-58-2**, Stentorin
RL: PRP (Properties)
(structural aspects and electronic absorption of hydroxyphenanthroperylene quinones fringelite D, hypericin, and stentorin)
RN 122194-30-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,13-tetrahydroxy- (9CI) (CA INDEX NAME)



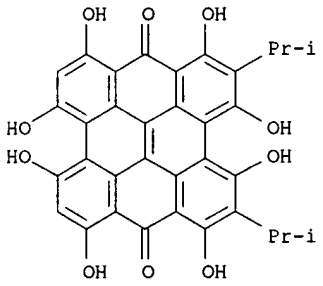
RN 141600-17-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6-dihydroxy- (9CI) (CA INDEX NAME)



RN 141600-18-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-dihydroxy- (9CI) (CA INDEX NAME)

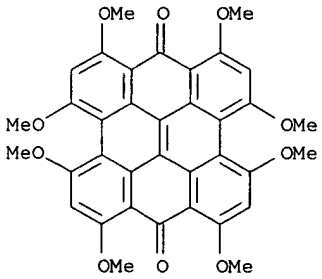


RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

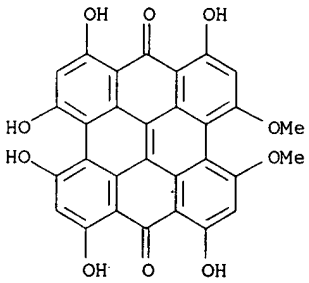


=> d bib abs hitstr l54 21

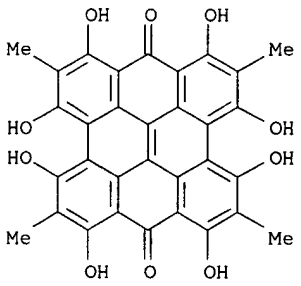
L54 ANSWER 21 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:545215 HCAPLUS
DN 125:275503
TI The synthesis and biological evaluation of hypericin analogs. [Erratum to document cited in CA124:55665]
AU Kraus, G. A.; Zhang, W.; Carpenter, S.; Wannemuehler, Y.
CS Dep. Chemistry, Iowa State Univ., Ames, IA, 50011, USA
SO Bioorg. Med. Chem. Lett. (1996), 6(16), 2037
CODEN: BMCLE8; ISSN: 0960-894X
DT Journal
LA English
AB The second full sentence on p. 2634 is cor. The errors were not reflected in the abstr. or the index entries.
IT **168287-28-3P 172226-96-9P 172226-97-0P**
172226-98-1P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and anti-retroviral activity of hypericin analogs (Erratum))
RN 168287-28-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octamethoxy- (9CI) (CA INDEX NAME)



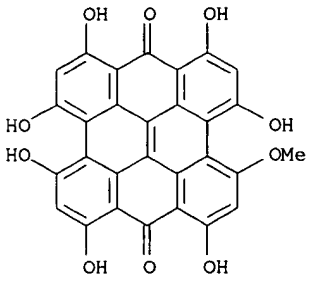
RN 172226-96-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy- (9CI) (CA INDEX NAME)



RN 172226-97-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5,9,12-tetramethyl- (9CI) (CA INDEX NAME)



RN 172226-98-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,13-heptahydroxy-11-methoxy- (9CI) (CA INDEX NAME)

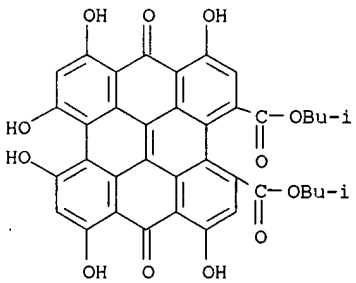

OH
O
OH
HO
OH
HO
OMe
OH
O
OH

=> d bib abs hitstr l54 22

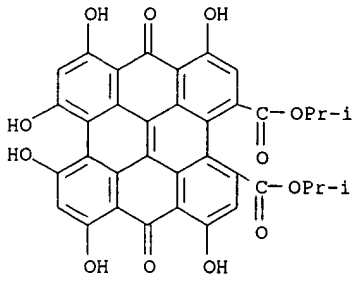
L54 ANSWER 22 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:340828 HCAPLUS
DN 125:2971
TI Delivery of nucleic acids to cells for transfection using hypericin-polyamine complexes
IN Lavie, Gad; Prince, Alfred M.
PA New York University, USA; New York Blood Center
SO PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9607731	A1	19960314	WO 1995-US11709	19950905
	W: AU, CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 5824654	A	19981020	US 1994-300725	19940902
	AU 9535894	A1	19960327	AU 1995-35894	19950905
PRAI	US 1994-300725		19940902		
	WO 1995-US11709		19950905		

OS MARPAT 125:2971
AB A method for transfection of cultured mammalian cell is provided. The cell is contacted with a complex of the nucleic acid with a hydrophobic, membrane-binding anion and a polycation. The hydrophobic anion may comprise a polycyclic arom. dione (such a hypericin or its analogs), an anthraquinone, an emodin anthrone deriv., a cercosporine deriv., or a fatty acid; the polycation may comprise polylysine, polyarginine, polyasparagine, or various polyalkyleneamines. Thus, a 36-mer oligodeoxyribonucleotide forms a complex with polylysine and hypericin. The complex is 40-50% assocd. with murine T-lymphoblastoid cells, whereas only .apprx.1% is assocd. when DNA was added to the cells in the absence of hypericin or polylysine. HIV p55 gag expression was inhibited in CEM cell cultures exposed to an antisense phosphorothioate oligonucleotide complexed with hypericin and polylysine, whereas the oligonucleotide alone, hypericin alone, and polylysine alone were relatively ineffective.
IT **177354-95-9 177354-96-0**
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(delivery of nucleic acids to cells for transfection using hypericin-polyamine complexes)
RN 177354-95-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)

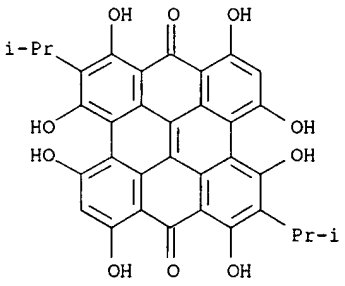


RN 177354-96-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)


OH
O
OH
HO
HO
C—OPr-i
O
C—OPr-i
O
OH
O
OH

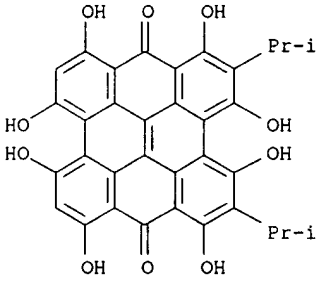
=> d bib abs hitstr l54 23

L54 ANSWER 23 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:308063 HCAPLUS
DN 125:29419
TI Bioorganic studies of a new photoreceptor structure
AU Orlando, M.; Gross, M. L.
CS MidWest Center Mass Spectrometry, University Nebraska, Lincoln, NE, 68588, USA
SO NATO ASI Ser., Ser. C (1996), 475(Mass Spectrometry in Biomolecular Sciences), 429-434
CODEN: NSCSDW; ISSN: 0258-2023
DT Journal
LA English
AB The aim of this work is to show the importance of using different instrumental techniques in the field of bioorg. research to det. the structure of unknown compds. present at trace levels in biol. systems. FAB MS and MS/MS were employed to elucidate structural features of a new type of photoreceptor chromophore. Moreover, a new approach for establishing the positions of OH groups in polyhydroxylated mols. has been developed, and the underlying ion chem. understood.
IT **147395-59-3**
RL: PRP (Properties)
(bioorg. studies of new photoreceptor structure stentorin)
RN 147395-59-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,9-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

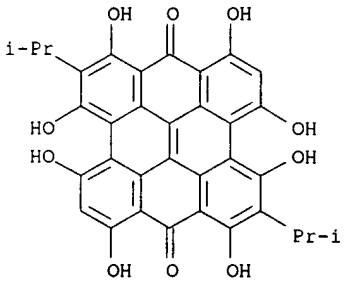


=> d bib abs hitstr l54 24

L54 ANSWER 24 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:64173 HCAPLUS
DN 124:175677
TI Syntheses, constitutions and properties of stentorin and isostentorin
AU Falk, H.; Mayr, E.
CS Institute Chemie, Johannes-Kepler Universitat, Linz, A-4040, Austria
SO Monatsh. Chem. (1995), 126(12), 1311-21
CODEN: MOCMB7; ISSN: 0026-9247
DT Journal
LA English
AB Stentorin and isostentorin were synthesized from 2-isopropyl-1,3,6,8-tetrahydroxyanthrone by dimerization and chromatog. sepn. of the resulting regioisomers. The anthrone was prepd. in 4 steps starting from easily available properly substituted benzene derivs.; the overall yield of the stentorins was 11%. The constitutions of stentorin and isostentorin could be unequivocally assigned from the 1H NMR spectra of their potassium salts and were found to be in agreement with those derived recently by means of a rational synthesis. The spectroscopic, dissocn., and acid-base properties in ground and excited states as well as the chiroptical properties of the human serum albumin complexes were investigated and discussed comparing them with resp. data of hypericin, fingelite D, and the natural Stentor pigment.
IT **147395-58-2P**, Stentorin **147395-59-3P**
173832-00-3P 173832-01-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(syntheses, mol. structures and properties of stentorin and isostentorin)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

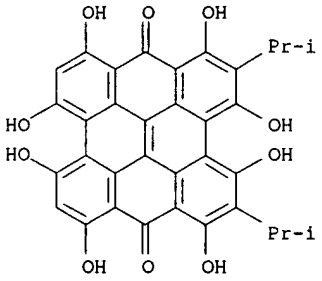


RN 147395-59-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,9-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)



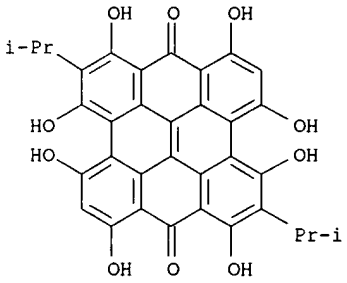
RN 173832-00-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, dipotassium salt, stereoisomer (9CI) (CA INDEX NAME)



●2 K

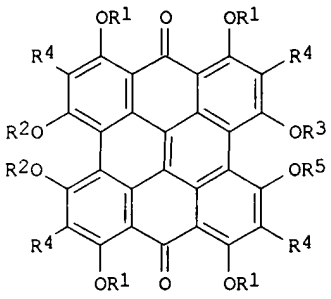
RN 173832-01-4 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,9-bis(1-methylethyl)-, dipotassium salt, stereoisomer (9CI) (CA INDEX NAME)



●2 K

=> d bib abs hitstr l54 25

L54 ANSWER 25 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:959345 HCAPLUS
DN 124:55665
TI The synthesis and biological evaluation of hypericin analogs
AU Kraus, George A.; Zhang, Weijiang
CS Dep. Chemistry, Iowa State Univ., Ames, IA, 50011, USA
SO Bioorg. Med. Chem. Lett. (1995), 5(22), 2633-6
CODEN: BMCLE8; ISSN: 0960-894X
DT Journal
LA English
GI

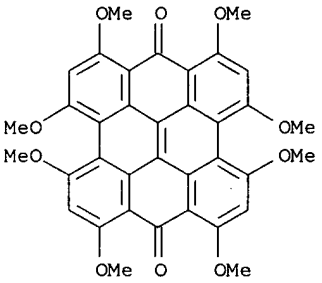


I

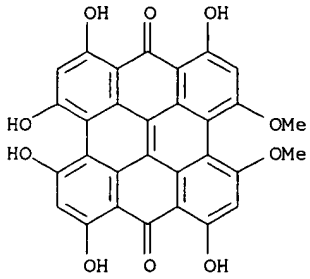
AB The hypericin analogs I [R1-R3, R5 = Me, R4 = H; R, R3-R5 = H, R2 = Me; R1-R5 = H; R1-R3, R5 = H, R4 = Me; R1, R2, R4, R5 = H, R3 = Me] were prepd. and tested for virucidal activity against equine infectious anemia virus. Although the peri-hydroxyl groups in hypericin are essential for retroviral inhibitory activity, the remaining hydroxyl groups can be alkylated without loss of activity.

IT **168287-28-3P 172226-96-9P 172226-97-0P**
172226-98-1P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and anti-retroviral activity of hypericin analogs)

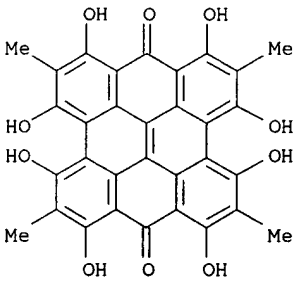
RN 168287-28-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octamethoxy- (9CI) (CA INDEX NAME)



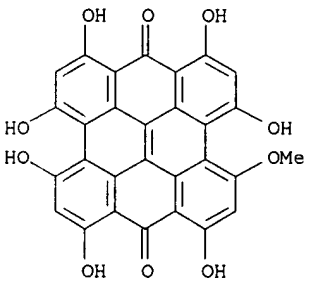
RN 172226-96-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy- (9CI) (CA INDEX NAME)



RN 172226-97-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5,9,12-tetramethyl- (9CI) (CA INDEX NAME)

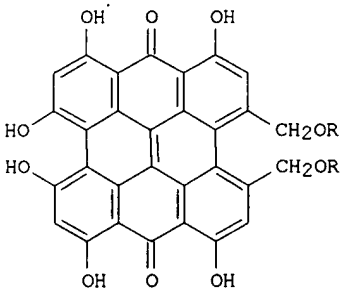


RN 172226-98-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,13-heptahydroxy-11-methoxy- (9CI) (CA INDEX NAME)



=> d bib abs hitstr l54 26

L54 ANSWER 26 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:946572 HCAPLUS
DN 124:29512
TI On the synthesis of .omega.-appended hypericin derivatives
AU Falk, H.; Vaisburg, A. F.; Amer, A. M.
CS Inst. Chemie, Johannes Kepler Univ., Linz, A-4040, Austria
SO Monatsh. Chem. (1995), 126(8/9), 993-1000
CODEN: MOCMB7; ISSN: 0026-9247
DT Journal
LA English
OS CASREACT 124:29512
GI

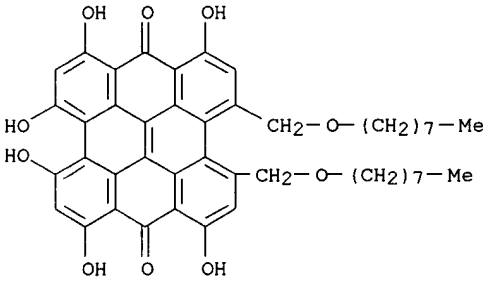


I

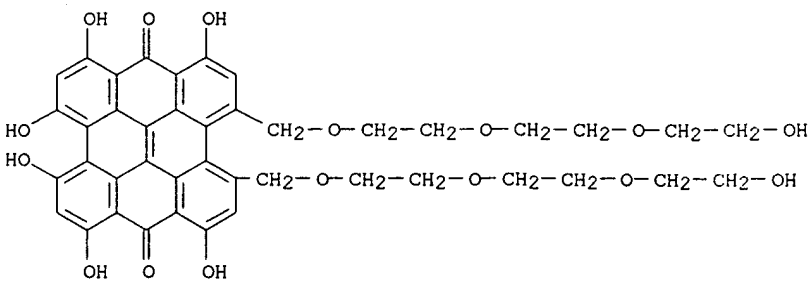
AB A method for the prepn. of bis-.omega.-appended hypericin derivs. I [R = octyl, hexadecyl, CH2CH2(OCH2CH2)2OH] was developed. The key step, the synthesis of appropriately .omega.-substituted emodin derivs., was achieved by solvolyzing 3-bromomethyl-1,6,8-triacetyloxy-anthracene-9,10-dione (.omega.-bromotriacetylemodin) in the appropriate alc. in the presence of silver perchlorate. I were then prepd. conventionally by dimerizing the .omega.-substituted emodin anthrones. The latter were prepd. by redn. of the .omega.-appended emodins. The soly of I is very similar to that of hypericin.

IT **171782-04-0P 171782-06-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of alkoxy-substituted hypericin)

RN 171782-04-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[(octyloxy)methyl]- (9CI) (CA INDEX NAME)

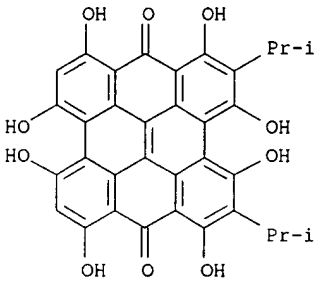


RN 171782-06-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]methyl]- (9CI) (CA INDEX NAME)



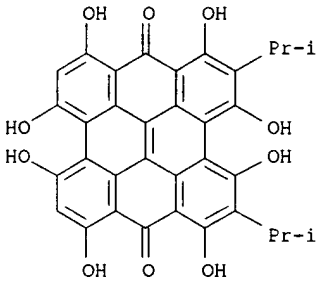
=> d bib abs hitstr l54 27

L54 ANSWER 27 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:882693 HCAPLUS
DN 123:313580
TI Photo-mechanical responses in the unicellular ciliates
AU Song, Pill Soon
CS Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588-0304, USA
SO Kagaku to Kogyo (Tokyo) (1995), 48(10), 1222-5
CODEN: KAKTAF; ISSN: 0022-7684
DT Journal; General Review
LA Japanese
AB A review with 6 refs. Photoreceptor structure and photochem. function of Stentor coeruleus and Blepharisma japonicum are discussed.
IT **147395-58-2**, Stentorin
RL: MSC (Miscellaneous)
(photomech. responses in unicellular ciliates)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)



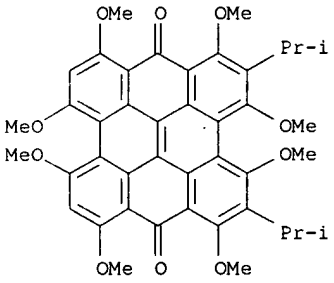
=> d bib abs hitstr l54 28

L54 ANSWER 28 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:775793 HCAPLUS
DN 123:169411
TI Spectroscopic characterization of hypericin and related compounds (stentorin)
AU Wynn, Jeanne Lenore
CS Iowa State Univ., Ames, IA, USA
SO (1994) 108 pp. Avail.: Univ. Microfilms Int., Order No.: DA9518458 From: Diss. Abstr. Int., B 1995, 56(2), 789
DT Dissertation
LA English
AB Unavailable
IT **147395-58-2**, Stentorin
RL: PRP (Properties)
(spectroscopic properties of stentorin in soln.)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

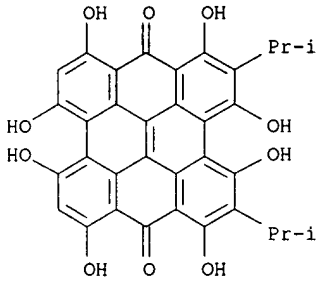


=> d bib abs hitstr l54 29

L54 ANSWER 29 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:760462 HCAPLUS
DN 123:198504
TI A facile synthesis of stentorin, the photoreceptor of Stentor coeruleus
AU Iio, Hideo; Zenfuku, Kazutaka; Tokoroyama, Takashi
CS Fac. Sci., Osaka City Univ., Osaka, 558, Japan
SO Tetrahedron Lett. (1995), 36(33), 5921-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 123:198504
AB Stentorin, a protozoan photoreceptor, was effectively synthesized via the Ullmann coupling reaction of 5-bromo-2-isopropyl-1,3,6,8-tetramethoxyanthraquinone, which was prepd. from 3-isopropyl-2,4-dimethoxy-6-(3,5-dimethoxybenzyl)benzoic acid via intramol. Friedel-Crafts reaction and regioselective bromination.
IT **167961-26-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of stentorin, the photoreceptor of Stentor coeruleus)
RN 167961-26-4 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octamethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

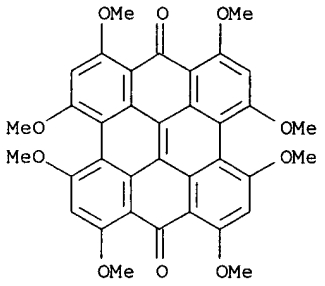


IT **147395-58-2P**, Stentorin
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of stentorin, the photoreceptor of Stentor coeruleus)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)



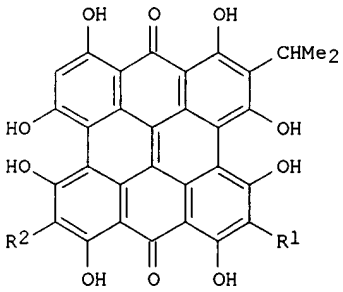
=> d bib abs hitstr l54 30

L54 ANSWER 30 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:758185 HCAPLUS
DN 123:202007
TI Synthesis and properties of fringelite D (1,3,4,6,8,10,11,13-octahydroxy-phenanthro[1,10,9,8,o,p,q,r,a]perylene-7,14-dione)
AU Falk, H.; Mayr, E.
CS Inst. Chem., Johannes Kepler Univ., Linz, A-4040, Austria
SO Monatsh. Chem. (1995), 126(6/7), 699-710
CODEN: MOCMB7; ISSN: 0026-9247
DT Journal
LA English
AB Fringelite D was synthesized from 1,3,6,8-tetramethoxyanthracen-9-ol via two different efficient routes. The first one involved demethylation and subsequent dimerization. The other one started with dimerization to yield octamethylfringelite D and subsequent demethylation. The starting material was prepd. in four steps from com. available educts, the key step being a benzamide ortho-lithiation. The spectroscopic properties of fringelite D were measured and are discussed. The dissocn., deprotonation, and protonation equil. of fringelite D were characterized by their resp. pK values in ground and excited states and compared with those of hypericin. Homo- and heteroassocn. properties of fringelite D were similar to those of hypericin.
IT **168287-28-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(intermediate; prepn. and properties of fringelite D pigment)
RN 168287-28-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octamethoxy- (9CI) (CA INDEX NAME)



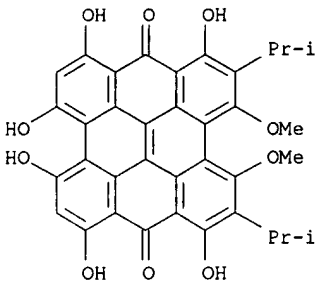
=> d bib abs hitstr l54 31

L54 ANSWER 31 OF 61 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:510603 HCAPLUS
DN 122:290569
TI Synthesis of Stentorin
AU Cameron, Donald W.; Riches, Andrew G.
CS School Chemistry, University Melbourne, Parville, Victoria, 3052, Australia
SO Tetrahedron Lett. (1995), 36(13), 2331-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
GI

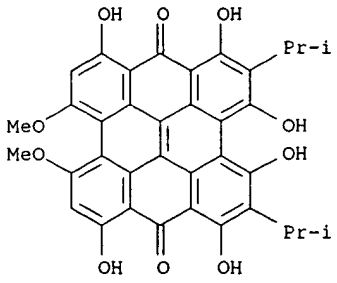


I

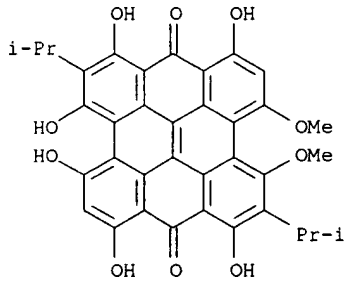
AB The two sym. naphthodianthrone structures I (R1 = CHMe2, R2 = H; R1 = H, R2 = CHMe2) proposed for the photodynamic pigment stentorin have both been synthesized, thereby establishing the correctness of structure I (R1 = CHMe2, R2 = H).
IT **162975-31-7P 162975-32-8P 162975-33-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of stentorin)
RN 162975-31-7 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,10,11,13-hexahydroxy-3,4-dimethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



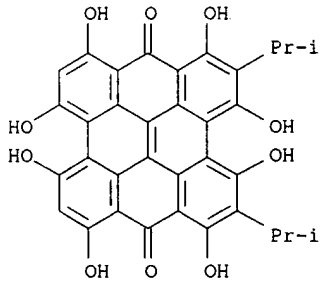
RN 162975-32-8 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



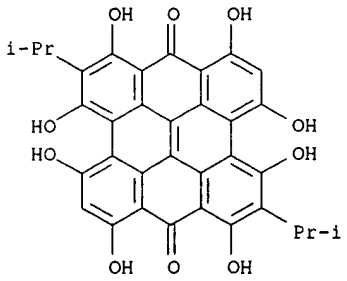
RN 162975-33-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-2,9-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



IT **147395-58-2P**, Stentorin **147395-59-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of stentorin)
RN 147395-58-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)



RN 147395-59-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,9-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)


OH
O
OH
i-Pr
HO
OH
HO
OH
Pr-i
OH
O
OH

=> d bib abs hitstr l7

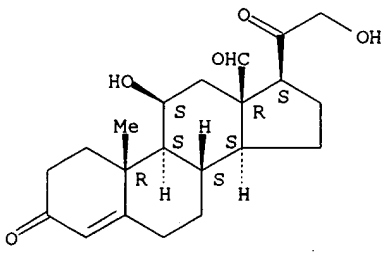
L7 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2000 ACS
AN 2000:53336 HCAPLUS
DN 132:88203
TI Hypericin, hypericin derivatives, and Hypericum extract as specific T-type calcium channel blockers, and their use as T-type calcium channel targeted therapeutics
IN **Shan, Jacqueline J.; Wu, Xi-Chen; Pang, Peter K. T.; Ling, Lei**
PA CV Technologies Inc., Can.
SO PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000002455	A1	20000120	WO 1999-US14132	19990709
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9949581	A1	20000201	AU 1999-49581	19990709

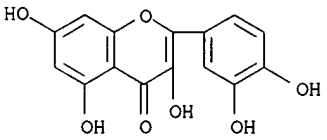
PRAI US 1998-92227 19980709
WO 1999-US14132 19990709
OS MARPAT 132:88203
AB Hypericin has been shown to specifically inhibit T-type calcium channel activity. Hypericum ext. contg. hypericin also inhibits T-type calcium channel activity. Moreover, other chems. in Hypericum ext. showed a synergistic effect to hypericin. In view of this, hypericin or hypericin-contg. Hypericum ext. can be used as T-channel blockers. Hypericum ext., ext. of other species of the Hypericum genus, ext. of other plants contg. hypericin, hypericin derivs., hypericin analogs, e.g. pseudohypericin, and other Hypericum ext. constituents can be used as therapeutics targeted at T-type calcium channels for treatment of diseases assocd. with T-channel abnormality. Methods for administering hypericin and Hypericum ext. are disclosed.
IT **9004-10-8**, Insulin, biological studies
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(hyper- and hypoinsulinemia; hypericin, derivs., and Hypericum ext. as specific T-type calcium channel blockers and use as T-type calcium channel targeted therapeutics)
RN 9004-10-8 HCAPLUS
CN Insulin (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **52-39-1**, Aldosterone
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(hyperaldosteronemia; hypericin, derivs., and Hypericum ext. as specific T-type calcium channel blockers and use as T-type calcium channel targeted therapeutics)
RN 52-39-1 HCAPLUS
CN Pregn-4-en-18-al, 11,21-dihydroxy-3,20-dioxo-, (11.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

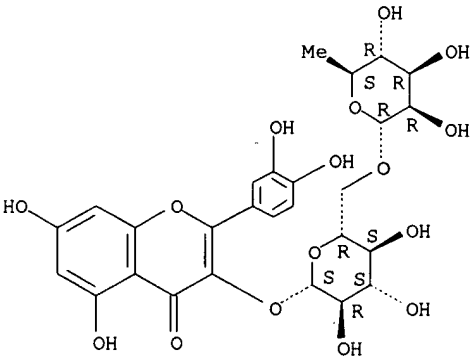


IT **117-39-5**, Quercetin **153-18-4**, Rutin **482-36-0**, Hyperoside **522-12-3**, Quercitrin **548-04-9**, Hypericin **548-04-9D**, Hypericin, derivs. and analogs **1617-53-4**, Amentoflavone **11079-53-1**, Hyperforin **21637-25-2**, Isoquercitrin **55954-61-5**, Pseudohypericin **143183-63-5**, Adhyperforin
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hypericin, derivs., and Hypericum ext. as specific T-type calcium channel blockers and use as T-type calcium channel targeted therapeutics)
RN 117-39-5 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy- (9CI) (CA INDEX NAME)



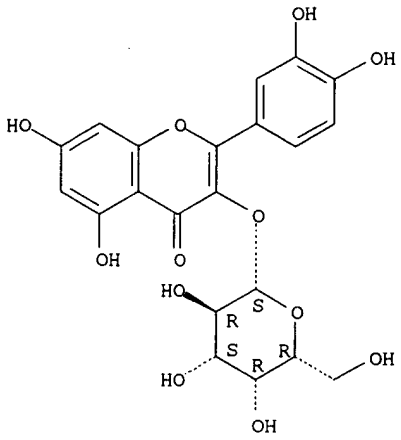
RN 153-18-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 3-[[6-O-(6-deoxy-.alpha.-L-mannopyranosyl)-.beta.-D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



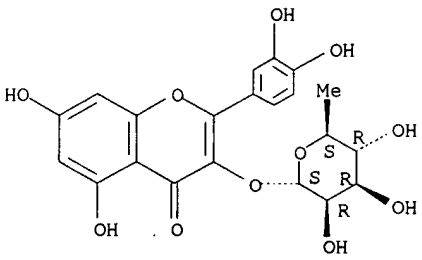
RN 482-36-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(.beta.-D-galactopyranosyloxy)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

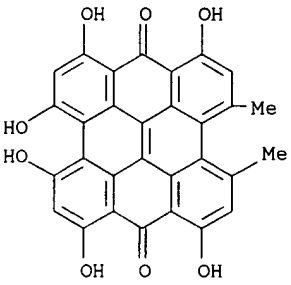


RN 522-12-3 HCAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(6-deoxy-.alpha.-L-mannopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

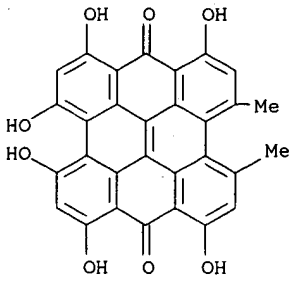
Absolute stereochemistry.



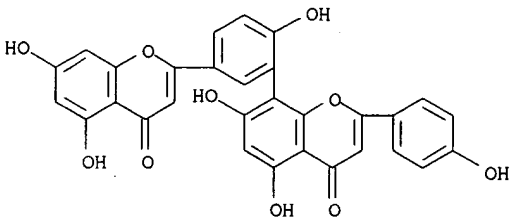
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

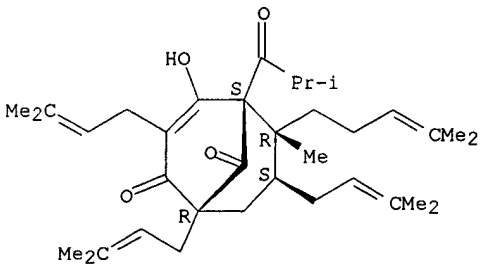


RN 1617-53-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 8-[5-(5,7-dihydroxy-4-oxo-4H-1-benzopyran-2-yl)-2-hydroxyphenyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



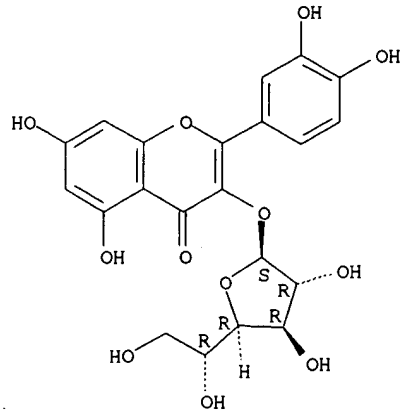
RN 11079-53-1 HCAPLUS
CN Bicyclo[3.3.1]non-3-ene-2,9-dione, 4-hydroxy-6-methyl-1,3,7-tris(3-methyl-2-butenyl)-5-(2-methyl-1-oxopropyl)-6-(4-methyl-3-pentenyl)-, (1R,5S,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

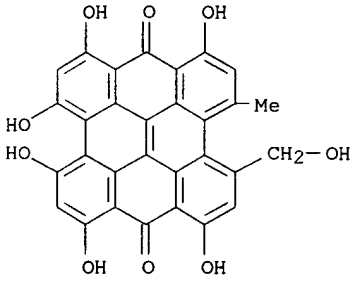


RN 21637-25-2 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(.beta.-D-glucofuranosyloxy)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

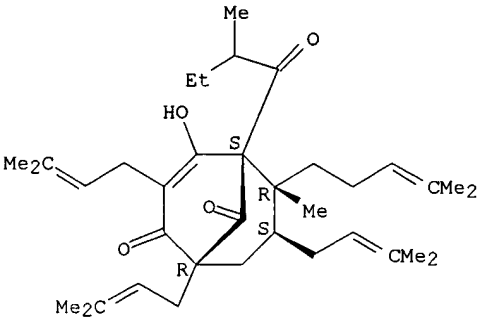


RN 55954-61-5 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-(hydroxymethyl)-11-methyl- (9CI) (CA INDEX NAME)



RN 143183-63-5 HCAPLUS
CN Bicyclo[3.3.1]non-3-ene-2,9-dione, 4-hydroxy-6-methyl-1,3,7-tris(3-methyl-2-butenyl)-5-(2-methyl-1-oxobutyl)-6-(4-methyl-3-pentenyl)-, (1R,5S,6R,7S)- (9CI) (CA INDEX NAME)

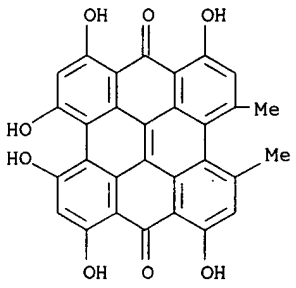
Absolute stereochemistry.



RE.CNT 3
RE
(1) Kikuta; US 5433957 A 1995
(2) Mazur; US 5120412 A 1992
(3) Noamesi; Planta Medica 1991, V57(Suppl 1), PA55

=> d bib abs hitstr l21 1

L21 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 2000:458255 HCAPLUS
TI Inhibition of human cytochrome P450 enzymes by constituents of St. John's wort, an herbal preparation used in the treatment of **depression**
AU Obach, R. Scott
CS Drug Metabolism Department, Candidate Synthesis, Enhancement, and Evaluation, Central Research Division, Pfizer, Inc., Groton, CT, USA
SO J. Pharmacol. Exp. Ther. (2000), 294(1), 88-95
CODEN: JPETAB; ISSN: 0022-3565
PB American Society for Pharmacology and Experimental Therapeutics
DT Journal
LA English
AB Com. available St. John's wort (Hypericum perforatum) exts., prepns. that are used in the treatment of **depression**, were examd. for the potential to inhibit human cytochrome P 450 (CYP) enzyme activities, specifically CYP1A2, CYP2C9, CYP2C19, CYP2D6, and CYP3A4. Crude exts. demonstrated inhibition of each of these five enzymes, with CYP2D6, CYP2C9, and CYP3A4 being more sensitive than CYP1A2 and CYP2C19. Exts. were fractionated by HPLC, and each of the fractions was tested for inhibition of these five CYPs to identify individual constituents with inhibitory activity. Several fractions were shown to possess inhibitory activity, including the fractions contg. hyperforin (the putative active antidepressant constituent), I3,II8-biapigenin, and hypericin. Hyperforin and I3,II8-biapigenin were isolated from the ext., and inhibition consts. for the five CYP activities were measured. In addn., three other constituents, hypericin, quercetin, and chlorogenic acid, were tested for inhibitory activity toward the CYP enzymes. The flavonoid compd. I3,II8-biapigenin was shown to be a potent, competitive inhibitor of CYP3A4, CYP2C9, and CYP1A2 activities with Ki values of 0.038, 0.32, and 0.95 .mu.M, resp. Hyperforin was a potent noncompetitive inhibitor of CYP2D6 activity (Ki = 1.5 .mu.M) and competitive inhibitor of CYP2C9 and CYP3A4 activities (Ki = 1.8 and 0.48 .mu.M, resp.). Hypericin also demonstrated potent inhibition of several CYP activities. These in vitro data indicate that St. John's wort prepns. contain constituents that can potently inhibit the activities of major human drug-metabolizing enzymes and suggest that these prepns. should be examd. for potential pharmacokinetic drug interactions in vivo.
IT **548-04-9**, Hypericin
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(inhibition of human cytochrome P 450 enzymes by constituents of St. John's wort)
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

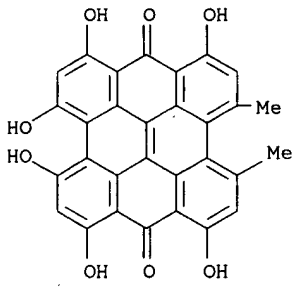


RE.CNT 23
RE
(1) Bailey, D; Br J Clin Pharmacol 1998, V46, P101 HCAPLUS
(4) Brolis, M; J Chromatogr A 1998, V825, P9 HCAPLUS
(5) Chan, K; J Label Compd Radiopharm 1982, V19, P321 HCAPLUS

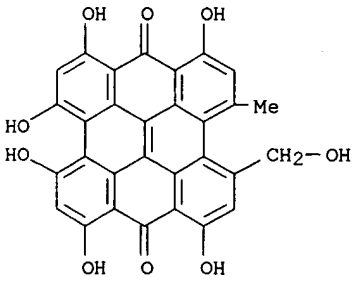
(7) deGroot, M; J Med Chem 1999, V42, P4062 HCAPLUS
(8) Edwards, D; Clin Pharmacol Ther 1999, V65, P237 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr l21 2

L21 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 2000:397036 HCAPLUS
DN 133:129833
TI Biochemical activities of extracts from hypericum perforatum L. 5th communication: dopamine-.beta.-hydroxylase-product quantification by HPLC and inhibition by hypericins and flavonoids
AU Denke, Andrea; Schempp, Harald; Weiser, Dieter; Elstner, Erich F.
CS Lehrstuhl fur Phytopathologie, Labor fur angewandte Biochemie, Technische Universitate Munchen, Freising-Weihenstephan, 85350, Germany
SO Arzneim.-Forsch. (2000), 50(5), 415-419
CODEN: ARZNAD; ISSN: 0004-4172
PB Editio Cantor Verlag
DT Journal
LA English
AB Exts. from the herb "St. John's wort" (Hypericum perforatum L.) exhibit beneficial effects on patients suffering from mental **depressions**. Lack of catecholamine neurotransmitters may be one biochem. mechanism for this problem under discussion. It has been recently reported that alc. exts. from Hypericum perforatum inhibit dopamine-.beta.-hydroxylase (D-.beta.-H) with an I50 or 0.1 .mu.mol/l on the basis of total hypericin content and with an I50 of 21 .mu.mol/l with pure com. hypericin. As test system polarog. detn. of oxygen uptake with tyramine as a substrate analog was used. In the present paper the quantification of the enzymic activity and the potential influence of inhibitors are reported using dopamine as substrate and product (noradrenaline) quantification by HPLC. With this test system it could be shown that D-.beta.-H is strongly inhibited by pseudohypericin (I50 = approx. 3 .mu.mol/l) and hypericin (I50 = approx. 5 .mu.mol/l), whereas the I50-values of various flavonoids (quercitrin, isoquercitrin, hyperoside, rutin, quercetin, amentoflavone, kaempferol) are in the range of 50 .mu.mol/l or higher.
IT **548-04-9**, Hypericin **55954-61-5**, Pseudohypericin
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(biochem. activities of exts. from hypericum perforatum and dopamine-.beta.-hydroxylase-product quantification by HPLC and inhibition by hypericins and flavonoids)
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 55954-61-5 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-(hydroxymethyl)-11-methyl- (9CI) (CA INDEX NAME)



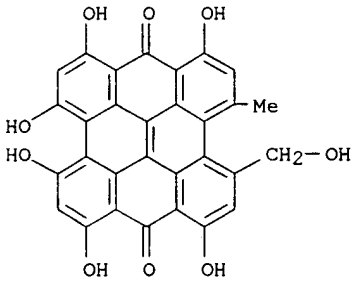
RE.CNT 13
RE
(1) Abdelnour-Esquivel, A; J Plant Growth Reg 1992, V11, P221 HCAPLUS
(2) Blouquit, M; Horm Metab Res 1996, V28, P122 MEDLINE
(3) de Paris, P; Biomed Environm Sci 1995, V8, P114 MEDLINE
(6) Fritze, J; Rev Neurosci 1993, V4, P63 MEDLINE
(10) Porter, J; Natural Toxins 1995, V3, P91 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr l21 3

L21 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 2000:362574 HCAPLUS
DN 132:343347
TI Methods and materials for treating **depression** and mood disorder with 5-hydroxytryptophan and an ext. of Hypericum perforatum or other extract and vitamins
IN Cho, Suk H.; Perkes, Lynn
PA Melaleuca, Incorporated, USA
SO U.S., 4 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6068846	A	20000530	US 1999-368789	19990805
PRAI US 1998-95378		19980805		

AB Methods and materials are provided for the treatment of **depression** or mood disorder. Specifically, the invention involves the use of 5-hydroxytryptophan and an ext. of e.g. Hypericum perforatum (St. John's Wort) to treat **depression** or mood disorders when administered orally. In addn., the invention provides less expensive, naturally derived dietary supplements to treat mild to moderate **depression** or mood disorder.
IT **55954-61-5**, Pseudohypericin
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(hydroxytryptophan and Hypericum perforatum ext. or other ext. and vitamins for treating **depression** and mood disorders)
RN 55954-61-5 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-(hydroxymethyl)-11-methyl- (9CI) (CA INDEX NAME)



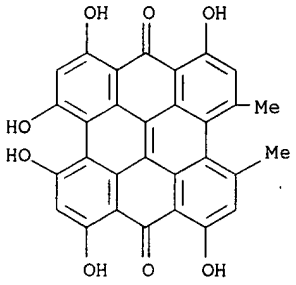
RE.CNT 3
RE
(1) Bewicke; US 5820867 1998
(2) Braswell; US 5911992 1999
(3) Laruelle; US 4472387 1984

=> d bib abs hitstr l21 4

L21 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 2000:277862 HCAPLUS
DN 132:298827
TI Natural composition for the treatment and prevention of **depression**, containing St. John's wort and folic acid derivatives.
IN Buchholz, Herwig; Dudda, Angela; Meduski, Jerzy
PA Merck Patent G.m.b.H., Germany
SO PCT Int. Appl., 13 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000023089	A1	20000427	WO 1999-EP7556	19991008
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI US 1998-104710		19981019		

AB A natural compn. comprises St. John's Wort (Hypericum perforatum L.), its exts. of active ingredients and derivs. of dihydro- and tetrahydrofolic acid. This natural formulation is useful for the treatment and prevention of **depression** with a better effect than the ingredients alone (no clin. data).
IT **548-04-9**, Hypericin
RL: **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(natural compn. for the treatment and prevention of **depression**, contg. St. John's wort and folic acid derivs.)
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RE.CNT 2
RE
(1) Bewicke, C; US 5820867 A 1998
(2) Nutramax Lab Inc; WO 9937155 A 1999

=> d bib abs hitstr l21 5

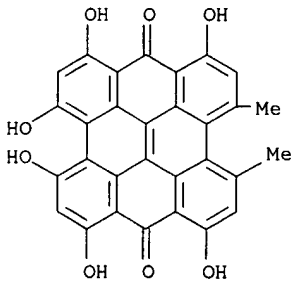
L21 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:819230 HCAPLUS
DN 132:44995
TI Neuroprotective composition for the prevention and/or treatment of nervous and behavioral alterations due to anxiety states or **depression**
IN Cavazza, Claudio
PA Sigma-Tau Healthscience S.p.A., Italy
SO PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9966914	A2	19991229	WO 1999-IT175	19990617
	WO 9966914	A3	20000406		
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9943910	A1	20000110	AU 1999-43910	19990617
PRAI	IT 1998-RM425		19980625		
	WO 1999-IT175		19990617		

AB A compn. is disclosed for the prevention and/or therapeutic treatment of nervous and behavioral alterations due to anxiety states or **depression** that may take the form of a dietary supplement, dietetic support or of an actual medicine which comprises as characterizing active ingredients acetyl L-carnitine and hypericin. Pharmacol. tests show that, while carnitines alone did not modify aggression latency times in mice treated with the, their use in combination with either Hypericum ext. of hypericin potentiates the redn. in aggression which the latter produce in mice. Pharmaceutical compns. contg. the combination were given.

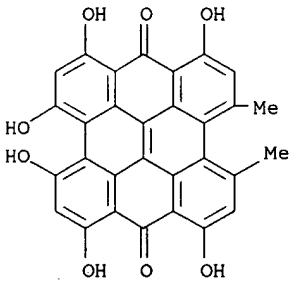
IT **548-04-9**, Hypericin
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(neuroprotective compn. for prevention and/or treatment of nervous and behavioral alterations due to anxiety states or **depression**)

RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



=> d bib abs hitstr l21 6

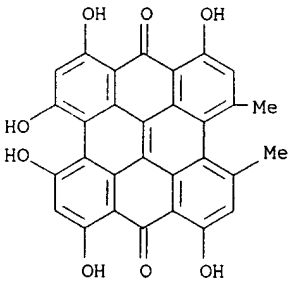
L21 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:468883 HCAPLUS
DN 131:120681
TI A double-blind randomized trial to investigate 3 different concentrations of a standardized fresh plant extract obtained from the shoot tips of Hypericum perforatum
AU Lenoir, S.; Degenring, F. H.; Saller, R.
CS St. Gallen, Switz.
SO Phytomedicine (1999), 6(3), 141-146
CODEN: PYTOEY; ISSN: 0944-7113
PB Urban & Fischer Verlag
DT Journal
LA English
AB The efficacy and tolerability was investigated of a new standardized fresh-plant ext. obtained from the shoot tips of St. John's wort (H. perforatum) in the treatment of mild to moderate **depression**. Out-patients with mild to moderate **depression** took during 6 wk 3 times a day 1 tablet of a Hypericum prepn. standardized to either 0.17, 0.33, or 1 mg total hypericin per day. The main outcome measure was the Hamilton Psychiatric Rating Scale for **Depression**. Addnl. measures were the Hospital Anxiety and **Depression** Scale and the Clin. Global Impression. At the end of treatment, a redn. in the av. Hamilton **Depression** score from an initial 16-17 to 8-9 was obsd. in all groups. The response rates were 62, 65, and 68%, resp. Tolerability was excellent, with mild adverse reactions probably causally related to the treatment occurring in only 2% of the patients. The Hypericum prepn. is effective in all 3 doses and is well tolerated.
IT **548-04-9**, Hypericin
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(dose-dependant antidepressant activity of a Hypericum prepn.)
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RE.CNT 25
RE
(2) Brockmoller, J; Pharmacopsychiatr 1997, V30, P94 HCAPLUS
(3) Cott, J; Pharmacopsychiatr 1997, V30, P108 HCAPLUS
(9) Hoffmann, J; Z Allg Med 1979, V55, P776 MEDLINE
(11) Kerb, R; Antimicrob Agents Chemother 1996, V40, P2087 HCAPLUS
(25) Wheatley, D; Pharmacopsychiatr 1997, V30, P77 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr l21 7

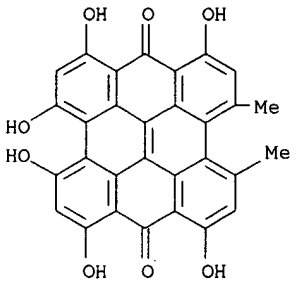
L21 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:87006 HCAPLUS
DN 130:144040
TI Hypericum for fatigue. A pilot study
AU Stevinson, Clare; Dixon, M.; Ernst, E.
CS Dep. Complementary Medicine, School Postgraduate Medicine Health Sciences, Univ. Exeter, Exeter, EX2 4NT, UK
SO Phytomedicine (1998), 5(6), 443-447
CODEN: PYTOEY; ISSN: 0944-7113
PB Gustav Fischer Verlag
DT Journal
LA English
AB Patients consulting their doctors complaining of fatigue were treated with Hypericum ext. (3 .times. 1 tablet daily) for 6 wk. Compared to baseline values, perceived fatigue was lower after 2 wk of treatment and reduced further after 6 wk. Symptoms of **depression** and anxiety were also reduced. Nearly half the sample was supposed to be depressed at the start of the trial which was possibly related to fatigue.
IT **548-04-9**, Hypericin
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(hypericum for fatigue)
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RE.CNT 9
RE
(1) Bowling, A; Measuring disease: a review of disease specific quality of life measurement scales 1996
(4) Linde, K; Br Med J 1996, V313, P253 MEDLINE
(6) Ridsdale, L; Brit J Gen Pract 1994, V44, P413 MEDLINE
(7) Shahar, E; J Fam Pract 1990, V31(3), P257 MEDLINE
(9) Zigmond, A; Acta Psychiat Scand 1983, V67, P361 MEDLINE
ALL CITATIONS AVAILABLE IN THE RE FORMAT

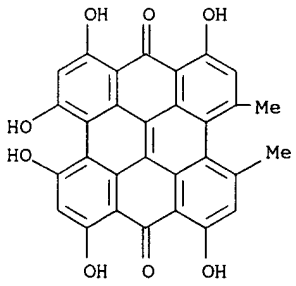
=> d bib abs hitstr l21 8

L21 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:738207 HCAPLUS
DN 128:43774
TI In vitro receptor binding and enzyme inhibition by Hypericum perforatum extract
AU Cott, J. M.
CS Pharmacologic Treatment Research Program, National Institute of Mental Health (NIMH), National Institutes of Health, Rockville, MD, USA
SO Pharmacopsychiatry (1997), 30(Suppl. 2), 108-112
CODEN: PHRMEZ; ISSN: 0176-3679
PB Thieme
DT Journal
LA English
AB Hypericum perforatum L. Hypericaceae (St. John's wort), has been used since the time of ancient Greece for its many medicinal properties. Modern usage is still quite diverse and includes wound healing, kidney and lung ailments, insomnia and **depression**. This plant has been known to contain a red pigment, hypericin, and similar compds., which have been assumed to be the primary active constituent(s) in this plant genus. A crude Hypericum ext. was tested in a battery of 39 in vitro receptor assays, and two enzyme assays. A sample of pure hypericin was also tested. Hypericin had affinity only for NMDA receptors while the crude ext. had significant receptor affinity for adenosine (nonspecific), GABAA, GABAB, benzodiazepine, inositol triphosphate, and monoamine oxidase (MAO) A and B. With the exception of GABAA and GABAB, the concns. of Hypericum exact required for these in vitro activities are unlikely to be attained after oral administration in whole animals or humans. These data are consistent with recent pharmacol. evidence suggesting that other constituents of this plant may be of greater importance for the reported psychotherapeutic activity. Alternative pharmacol. mechanisms for Hypericum's antidepressant activity are critically reviewed and the possible importance of GABA receptor binding in the pharmacol. of Hypericum is highlighted. Some of these results have been previously reported (Cott, 1995; Cott, 1996; Cott and Misra, 1997).
IT **548-04-9**, Hypericin
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(receptor binding and enzyme inhibition by Hypericum perforatum ext.)
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

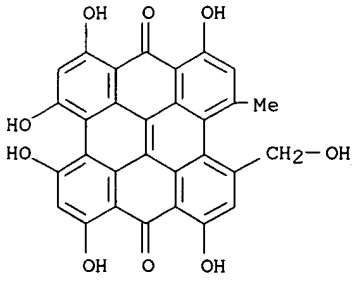


=> d bib abs hitstr l21 9

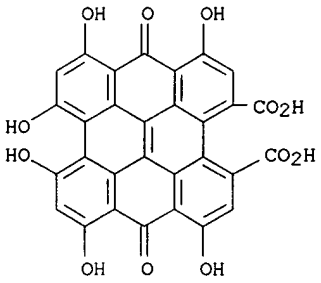
L21 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:226504 HCAPLUS
DN 124:311186
TI A comparative analysis of the photosensitized inhibition of growth-factor regulated protein kinases by hypericin-derivatives
AU Agostinis, P.; Donella-Deana, A.; Cuveele, J.; Vandenbogaerde, A.; Sarno, S.; Merlevede, W.; de Witte, P.
CS Afdeling Biochemie, Katholieke Universiteit, Louvain, Belg.
SO Biochem. Biophys. Res. Commun. (1996), 220(3), 613-17
CODEN: BBRCA9; ISSN: 0006-291X
DT Journal
LA English
AB The photodynamic inhibitory effect of hypericin and a no. of hypericin-derivs. were investigated in vitro using numerous growth-factor regulated protein kinases including receptor-bound (**Insulin**-R, EGF-R) and non-receptor (Lyn, c-Fgr, CSK, Syk) protein tyrosine kinases as well as Ser/Thr (PK-C, protein kinase CK-2, CK-1) protein kinases. Modification of the hypericin structure altered significantly the specificity of the protein kinase inhibition. In particular, methylation or attachment of long lipophilic chains to both Me groups of the hypericin mol. strongly enhanced the specificity toward PK-C.
IT **548-04-9**, Hypericin **55954-61-5**, Pseudohypericin **60483-14-9**, Hypericin dicarboxylic acid **120667-79-0** **137363-72-5**, Gymnochrome B **147593-87-1**, 2,5-Dibromohypericin **147593-89-3**, 2,5,9,12-Tetrabromohypericin **157301-83-2**, Fringelite D **171782-05-1**
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(photosensitized inhibition of growth-factor regulated protein kinases by hypericin derivs.: comparative anal.)
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



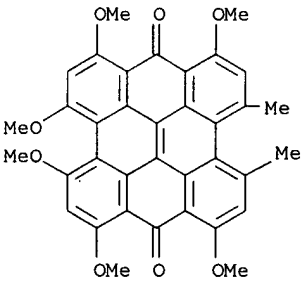
RN 55954-61-5 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-(hydroxymethyl)-11-methyl- (9CI) (CA INDEX NAME)



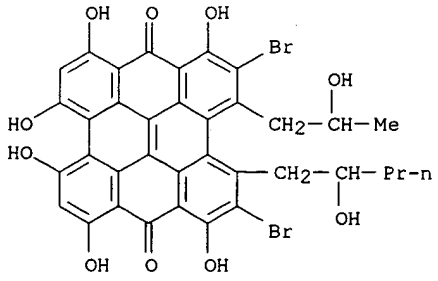
RN 60483-14-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo- (9CI) (CA INDEX NAME)



RN 120667-79-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME)

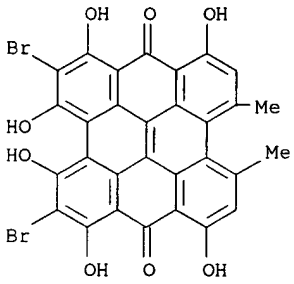


RN 137363-72-5 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,9,12-tribromo-1,3,4,6,8,13-hexahydroxy-10(or 11)-(2-hydroxypentyl)-11(or 10)-(2-hydroxypropyl)-, stereoisomer (9CI) (CA INDEX NAME)

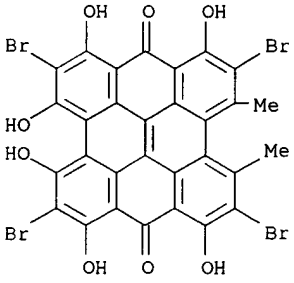


D1—Br

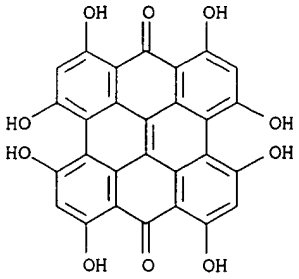
RN 147593-87-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dibromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)



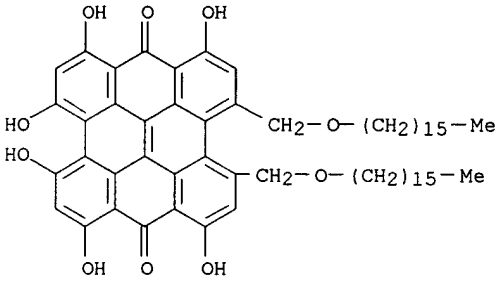
RN 147593-89-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5,9,12-tetrabromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)



RN 157301-83-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy- (9CI) (CA INDEX NAME)

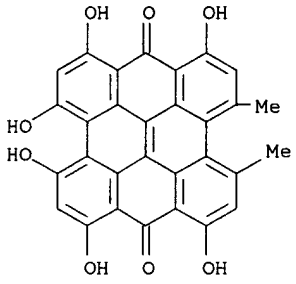


RN 171782-05-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis[(hexadecyloxy)methyl]-1,6,8,10,11,13-hexahydroxy- (9CI) (CA INDEX NAME)



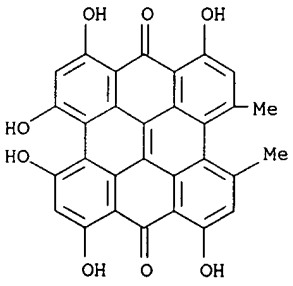
=> d bib abs hitstr l21 10

L21 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:620220 HCAPLUS
DN 123:51258
TI Photosensitized inhibition of growth factor-regulated protein kinases by hypericin
AU Agostinis, P.; Vandenbogaerde, A.; Donnella-Deana, A.; Pinna, L. A.; Lee, K.-T.; Goris, J.; Merlevede, W.; Vandenheede, J. R.; De Witte, P.
CS Fac. Farmaceutische Wetenschappen, Katholieke Univ. Leuven, Belg.
SO Biochem. Pharmacol. (1995), 49(11), 1615-22
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB The naphthodianthrone hypericin causes a photosensitized inhibition of protein kinases involved in growth factor signaling pathways. Nanomolar concns. of hypericin inhibit the protein tyrosine kinase activities (PTK) of the epidermal growth factor receptor and the **insulin** receptor, while being ineffective towards the cytosolic protein tyrosine kinases Lyn, Fgr, TPK-IIB and CSK. Photosensitized inhibition by hypericin is not restricted to receptor-PTKs since the Ser/Thr protein kinases (protein kinase CK-2, protein kinase C and mitogen-activated kinase) are also extremely sensitive to inhibition (IC50 value for protein kinase CK-2=6 nM). A comparison of the hypericin-mediated inhibition of the epidermal growth factor-receptor PTK and protein kinase CK-2 revealed that the inhibition is irreversible, strictly dependent upon irradn. of the enzyme-inhibitor complex with fluorescent light and likely mediated by the formation of radical intermediates (type I mechanism). Although the exact mol. basis for the selectivity of enzyme inhibition by hypericin remains unknown, the results suggest that distinctly related protein kinases could still share common reactive domains for the interaction with hypericin.
IT **548-04-9**, Hypericin
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(photosensitized inhibition of growth factor-regulated protein kinases by hypericin)
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



=> d bib abs hitstr l21 11

L21 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN 1987:113450 HCAPLUS
DN 106:113450
TI Experimental animal studies of the psychotropic activity of a Hypericum extract
AU Okpanyi, S. N.; Weischer, M. L.
CS Inst. Pharmakol. Toxikol., Univ. Muenster, Muenster, 4400, Fed. Rep. Ger.
SO Arzneim.-Forsch. (1987), 37(1), 10-13
CODEN: ARZNAD; ISSN: 0004-4172
DT Journal
LA German
AB Exts. of H. perforatum (Psychotonin M) with known concns. of hypericin [548-04-9] were tested in animal models used for screening psychotropics, and in particular of antidepressant activity. Hypericum Ext. enhanced the exploratory activity of mice in a foreign environment dose-dependently prolonged the narcotic sleeping time, and within a narrow dose range exhibited reserpine antagonism. Similar to most other antidepressants, Hypericum ext. enhanced the activity of mice in the water-wheel test and after a prolonged daily administration decreased aggressiveness in socially isolated male mice. This data in addn. to the already proven clin. efficacy justify the use of standardized Hypericum ext. in the treatment of mild to moderate **depression**.
IT **548-04-9**, Hypericin
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(of Hypericum perforatum ext., antidepressant activity of)
RN 548-04-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

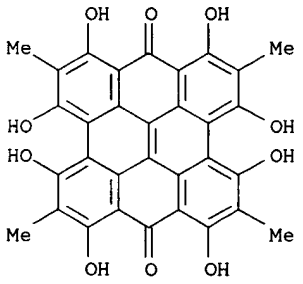


=> d bib abs hitstr 153

L53 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:487842 HCAPLUS
DN 129:119683
TI Photoactivated antiviral and antitumor compositions
IN Kraus, George A.; Carpenter, Susan L.; Petrich, Jacob W.
PA Iowa State University Research Foundation, USA
SO U.S., 26 pp. Cont.-in-part of U.S. Ser. No. 995,887, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

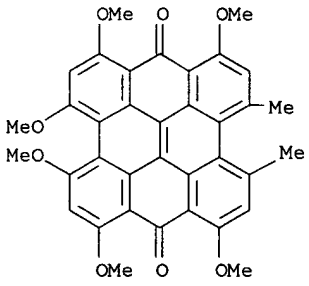
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5780287	A	19980714	US 1995-474000	19950607
PRAI US 1992-995877		19921223		

OS MARPAT 129:119683
AB Disclosed herein are compds., compns., and methods to inactivate a virus and destroy tumor cells. The methods involve the addn. into the cell of a compd. contg. a photosensitizing chem. and an energy-donating chem., optionally linked by a chem. tether. Also introduced into the cell are means to chem. activate the energy-donating chem. which photoactivates the photosensitizing chem. which then destroys the tumor or virus. The photosensitizing chem. is preferably hypericin, porphyrin, or an analog and the energy-donating chem. is preferably luciferin or an analog. Methods for synthesizing the chems. are also disclosed. Further, the energy-donating chem. is activated by an activating chem. The expression of the activating chem. is regulated so as to target the virus-infected or tumor cells. Regulating the activating chem. is accomplished by a no. of methods including construction of an expression plasmid contg. a gene encoding the activating chem. under control of a promoter which is transactivated by replication of the virus or transactivated by elevated levels of proteins expressed in tumor cells.
IT **172226-97-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(photoactivated antiviral and antitumor compns.)
RN 172226-97-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5,9,12-tetramethyl- (9CI) (CA INDEX NAME)

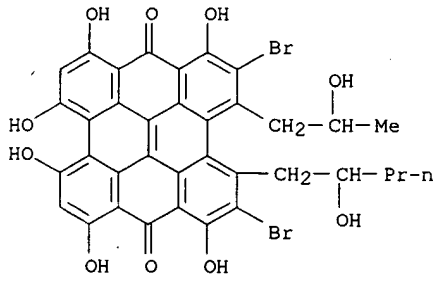


=> d bib abs hitstr l35 1

L35 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:729276 HCAPLUS
DN 132:32711
TI Bromohypericins are potent photoactive antiviral agents
AU Hudson, Jim B.; Delaey, Els; De Witte, Peter A.
CS Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, BC, V5Z 1M9, Can.
SO Photochem. Photobiol. (1999), 70(5), 820-822
CODEN: PHCBAP; ISSN: 0031-8655
PB American Society for Photobiology
DT Journal
LA English
AB Several hypericin derivs., previously shown to have interesting light-mediated biol. activities, were evaluated for antiviral activities against herpes simplex virus and influenza virus. Three brominated hypericins, the dibromo- and tetrabromo-derivs. and the natural compd. gymnochrome B were all very active against both viruses, particularly herpes simplex virus, although light was required in all cases for max. activity. The dibromohypericin was the most potent, under std. assay conditions, gymnochrome B was approx. as active as hypericin itself and tetrabromohypericin significantly less so. Surprisingly, hexamethylhypericin, which is known to have potent anti-protein kinase (PK) C activity, as well as anticell proliferation properties, showed no antiviral activity at all. The compds. were also evaluated in different serum concns. All the active compds. were inhibited by increasing concns. of serum, but to different degrees, such that their relative antiviral potencies changed to some extent. Thus, in summary, there was no correlation between antiviral and anti-PK or anticellular activities, and consequently it is not possible at present to define those structural features of hypericin-type mols. that are required for their various biol. activities.
IT **120667-79-0 137363-72-5,** Gymnochrome B
147593-87-1 147593-89-3
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(bromohypericins as photoactive antiviral agents)
RN 120667-79-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME)

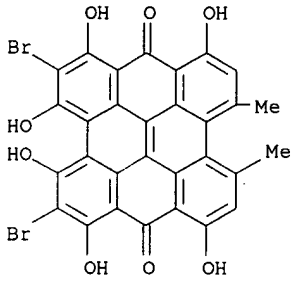


RN 137363-72-5 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,9,12-tribromo-1,3,4,6,8,13-hexahydroxy-10(or 11)-(2-hydroxypentyl)-11(or 10)-(2-hydroxypropyl)-, stereoisomer (9CI) (CA INDEX NAME)

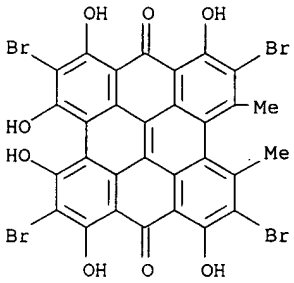


Dl—Br

RN 147593-87-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dibromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)



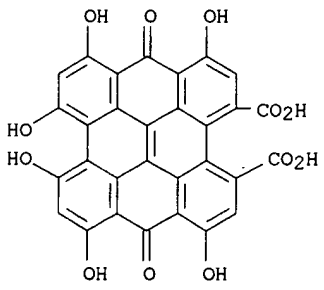
RN 147593-89-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5,9,12-tetrabromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)



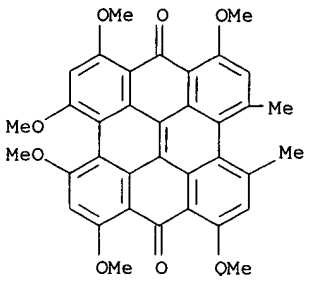
RE.CNT 10
RE
(2) Carpenter, S; Photochem Photobiol 1991, V53, P169 HCAPLUS
(3) Hudson, J; Antiviral Res 1991, V15, P101 HCAPLUS
(4) Hudson, J; Antiviral Res 1993, V20, P173 HCAPLUS
(5) Hudson, J; Photochem Photobiol 1997, V65, P352 HCAPLUS
(6) Hudson, J; Planta Med 1994, V60, P329 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr l35 2

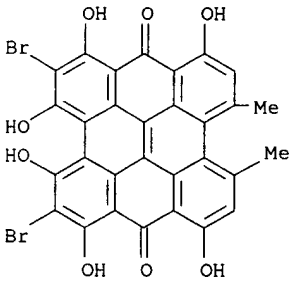
L35 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:68186 HCAPLUS
DN 128:215036
TI Cytotoxicity and antiproliferative effect of hypericin and derivatives after photosensitization
AU Vandenbogaerde, Ann L.; Delaey, Els M.; Vantieghem, Annelies M.; Himpens, Bernard E.; Merlevede, Wilfried J.; De Witte, Peter A.
CS Laboratorium voor Farmaceutische Biologie en Fytofarmacologie, Faculteit Farmaceutische Wetenschappen, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SO Photochem. Photobiol. (1998), 67(1), 119-125
CODEN: PHCBAP; ISSN: 0031-8655
PB American Society for Photobiology
DT Journal
LA English
AB The toxicity on three human tumor cell lines (A431, HeLa and MCF7) of five phenanthroperylenequinones (hypericin and derivs.) and two perylenequinones (cercosporin and calphostin C) was investigated after photosensitization (4 J/cm2). Furthermore, the antiproliferative effect on HeLa cells was studied for the phenanthroperylenequinones. Hypericin, 2,5-dibromohypericin, 2,5,9,12-tetrabromohypericin and perylenequinones displayed a potent cytotoxic and antiproliferative effect in the nanomolar range. Hypericin dicarboxylic acid exhibited no photoactivity. In general, the antiproliferative activity correlated well with the photocytotoxicity. However, the nonphotocytotoxic compd. hexamethylhypericin showed potent antiproliferative activity in the nanomolar range, probably exerting its action by protein kinase C inhibition. Without light irradn., no cytotoxic and antiproliferative effect was obsd. for any photocytotoxic phenanthroperylenequinone compd. Furthermore, confocal laser microscopy revealed that the subcellular localization in A431 cells was similar for the photoactive compds.; the photosensitizers were mainly concd. in the perinuclear region, probably corresponding with the Golgi app. and the endoplasmic reticulum. In addn., the accumulation of the photosensitizers in HeLa cells was investigated. All compds. except hypericin dicarboxylic acid were found to conc. to a large extent in the cells. The compd. 2,5,9,12-tetrabromohypericin seemed intrinsically more effective than hypericin since the intracellular concn. of the bromoderivative was a magnitude of order lower than that of hypericin although both compds. showed similar photobiol. activity.
IT **60483-14-9**, Hypericin dicarboxylic acid **120667-79-0** **147593-87-1**, 2,5-Dibromohypericin **147593-89-3**, 2,5,9,12-Tetrabromohypericin
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); PRP (Properties); **THU (Therapeutic use)**; BIOL (Biological study); PROC (Process); USES (Uses)
(cytotoxicity and antiproliferative effect of hypericin and derivs. after photosensitization)
RN 60483-14-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo- (9CI) (CA INDEX NAME)



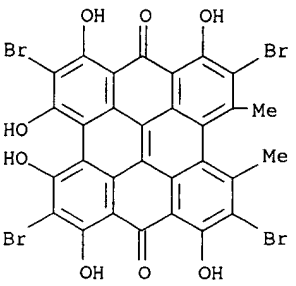
RN 120667-79-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME)



RN 147593-87-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dibromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

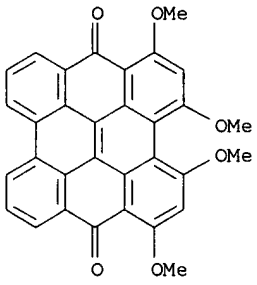


RN 147593-89-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5,9,12-tetrabromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

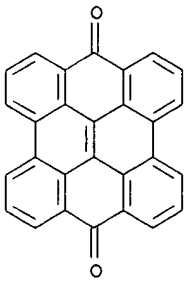


=> d bib abs hitstr l35 3

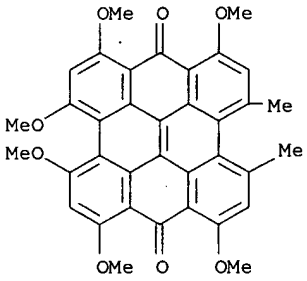
L35 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1997:247932 HCAPLUS
DN 126:303226
TI Hypericin, Hypocrellin, and Model Compounds: Primary Photoprocesses of Light-Induced Antiviral Agents
AU English, D. S.; Das, K.; Zenner, J. M.; Zhang, W.; Kraus, G. A.; Larock, R. C.; Petrich, J. W.
CS Department of Chemistry, Iowa State University, Ames, IA, 50011, USA
SO J. Phys. Chem. A (1997), 101(18), 3235-3240
CODEN: JPCAFH; ISSN: 1089-5639
PB American Chemical Society
DT Journal
LA English
AB The excited-state photophysics of the light-induced antiviral agents hypericin and hypocrellin are compared with those of the hexa- and tetramethoxy analogs of hypericin. The results are consistent with the interpretation of the primary photoprocess in hypericin and hypocrellin as that of excited-state intramol. proton or atom transfer.
IT **189113-18-6P**
RL: PRP (Properties); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(hypericin, hypocrellin, and model compds.: primary photoprocesses of light-induced antiviral agents)
RN 189113-18-6 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6-tetramethoxy- (9CI) (CA INDEX NAME)



IT **475-64-9 120667-79-0**
RL: PRP (Properties); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(hypericin, hypocrellin, and model compds.: primary photoprocesses of light-induced antiviral agents)
RN 475-64-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

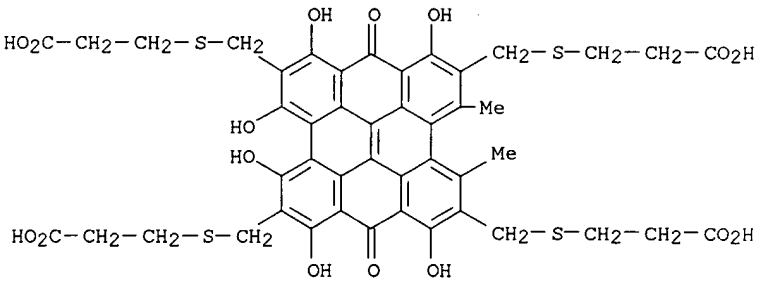


RN 120667-79-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME)



=> d bib abs hitstr l35 4

L35 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:664254 HCAPLUS
DN 126:84127
TI Antivirial activity of a derivative of the photosensitive compound hypericin
AU Yip, L.; Hudson, J. B.; Gruszecka-Kowalik, E.; Zalkow, L. H.; Towers, G. H. Neil
CS Dep. Botany, Univ. British Columbia, Vancouver, BC, Can.
SO Phytomedicine (1996), 3(2), 185-190
CODEN: PYTOEY; ISSN: 0944-7113
PB Fischer
DT Journal
LA English
AB Eight synthetic compds. related to the photosensitive antiviral quinonic plant compd. hypericin were screened for light-mediated antiviral activity. 2,5,9,12-Tetra(carboxyethylthiomethyl)hypericin showed activity against membrane-enveloped Sindbis virus and murine cytomegalovirus. The mechanism of action was of the photosensitive singlet oxygen type and the activity could be reduced by the presence of a singlet oxygen quencher mol.
IT **185672-52-0**
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(antiviral activity of photosensitive hypericin deriv.)
RN 185672-52-0 HCAPLUS
CN Propanoic acid, 3,3',3'',3'''-[(7,14-dihydro-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl-7,14-dioxophenanthro[1,10,9,8-opqra]perylene-2,5,9,12-tetrayl)tetrakis(methylenethio)]tetrakis- (9CI) (CA INDEX NAME)



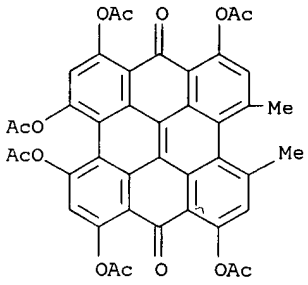
=> d bib abs hitstr l35 5

L35 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:333058 HCAPLUS
DN 125:26266
TI Methods and polycyclic aromatic compound containing compositions for treating T-cell-mediated diseases
IN Meruelo, Daniel; Lavie, Gad
PA New York University, USA
SO U.S., 21 pp. Cont.-in-part of U.S. Ser. No. 784, 952, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5514714	A	19960507	US 1993-39790	19930330
PRAI US 1990-572085		19900823		
US 1991-784952		19911101		

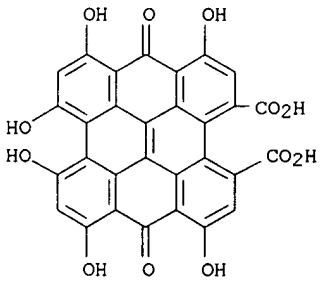
AB T cell-mediated diseases in mammals are treated using compns. comprising a polycyclic arom. compd., preferably hypericin or pseudohypericin, and related compds., including isomers, analogs, derivs., salts, or ion pairs of hypericin or pseudohypericin. The above compn. may be administered in combination with an immunosuppressive agent. Pharmaceutical compns. useful for treating a T cell-mediated disease comprise the above polycyclic arom. compd., alone or in combination with an immunosuppressive agent. The compns. and methods are useful in treating diseases which include multiple sclerosis, myasthenia gravis, scleroderma, polymyositis, graft-vs.-host disease, graft rejection, Graves disease, Addison's disease, autoimmune uveoretinitis, autoimmune thyroiditis, pemphigus vulgaris, psoriasis, systemic lupus erythematosus, and rheumatoid arthritis. Also provided are methods for diminishing the expression of CD4 Mols. on the surface of a T lymphocyte, and for inducing multidrug resistance in a cell, comprising incubating the cell with an effective concn. of a polycyclic arom. compd.

IT **55914-74-4**, Hypericin hexaacetate
RL: **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(polycyclic arom. compds. for treating T-cell-mediated diseases)
RN 55914-74-4 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexakis(acetyloxy)-10,11-dimethyl- (9CI) (CA INDEX NAME)

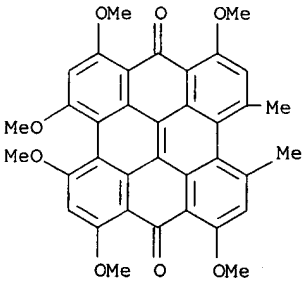


=> d bib abs hitstr l35 6

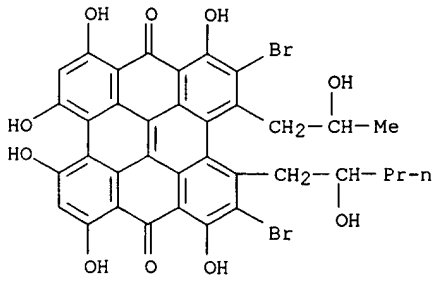
L35 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:226504 HCAPLUS
DN 124:311186
TI A comparative analysis of the photosensitized inhibition of growth-factor regulated protein kinases by hypericin-derivatives
AU Agostinis, P.; Donella-Deana, A.; Cuveele, J.; Vandenbogaerde, A.; Sarno, S.; Merlevede, W.; de Witte, P.
CS Afdeling Biochemie, Katholieke Universiteit, Louvain, Belg.
SO Biochem. Biophys. Res. Commun. (1996), 220(3), 613-17
CODEN: BBRCA9; ISSN: 0006-291X
DT Journal
LA English
AB The photodynamic inhibitory effect of hypericin and a no. of hypericin-derivs. were investigated in vitro using numerous growth-factor regulated protein kinases including receptor-bound (Insulin-R, EGF-R) and non-receptor (Lyn, c-Fgr, CSK, Syk) protein tyrosine kinases as well as Ser/Thr (PK-C, protein kinase CK-2, CK-1) protein kinases. Modification of the hypericin structure altered significantly the specificity of the protein kinase inhibition. In particular, methylation or attachment of long lipophilic chains to both Me groups of the hypericin mol. strongly enhanced the specificity toward PK-C.
IT **60483-14-9**, Hypericin dicarboxylic acid **120667-79-0** **137363-72-5**, Gymnochrome B **147593-87-1**, 2,5-Dibromohypericin **147593-89-3**, 2,5,9,12-Tetrabromohypericin **157301-83-2**, Fringelite D **171782-05-1**
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(photosensitized inhibition of growth-factor regulated protein kinases by hypericin derivs.: comparative anal.)
RN 60483-14-9 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo- (9CI) (CA INDEX NAME)



RN 120667-79-0 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME)

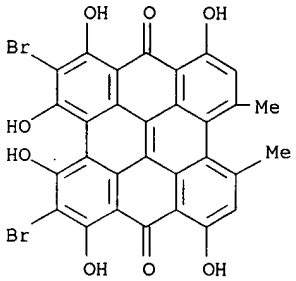


RN 137363-72-5 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,9,12-tribromo-1,3,4,6,8,13-hexahydroxy-10(or 11)-(2-hydroxypentyl)-11(or 10)-(2-hydroxypropyl)-, stereoisomer (9CI) (CA INDEX NAME)

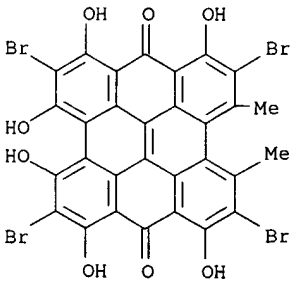


D1—Br

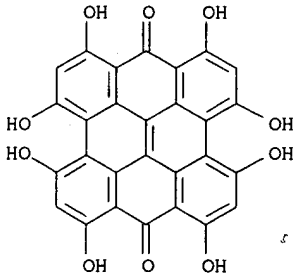
RN 147593-87-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dibromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)



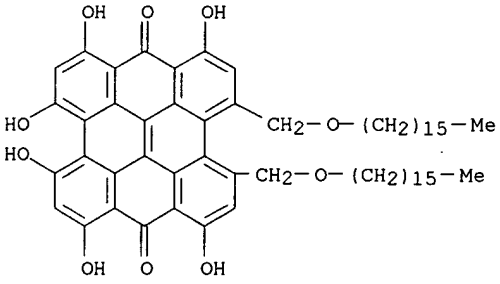
RN 147593-89-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5,9,12-tetrabromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)



RN 157301-83-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy- (9CI) (CA INDEX NAME)

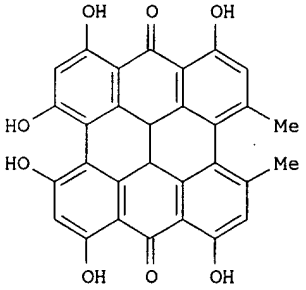


RN 171782-05-1 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis[(hexadecyloxy)methyl]-1,6,8,10,11,13-hexahydroxy- (9CI) (CA INDEX NAME)

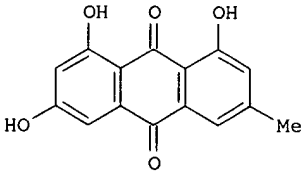


=> d bib abs hitstr 135 7

L35 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:185233 HCAPLUS
DN 124:284089
TI Antiviral activities of anthraquinones, bianthrones and hypericin derivatives from lichens
AU Cohen, P. A.; Hudson, J. B.; Toweres, G. H. N.
CS Dep. Botany, Univ. British Columbia, Vancouver, BC, V6T 1Z4, Can.
SO Experientia (1996), 52(2), 180-3
CODEN: EXPEAM; ISSN: 0014-4754
DT Journal
LA English
GI



I

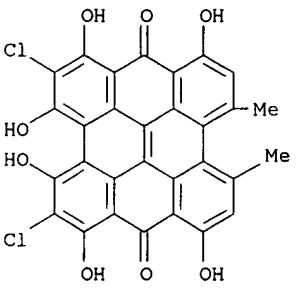


II

AB The antiviral activities of some naturally occurring anthraquinones, bianthrones, and hypericin derivs. were compared by the end-point CPE (viral cytopathic effects) method and plaque assays. Under optimal conditions of exposure to light, hypericin (I), 7,7'-dichloroemodin, and 5,7-dichloroemodin exhibited strong inhibitory activity against HSV-1 (herpes simplex virus type 1) in both assays. Partial inactivation of the virus was shown by emodin (II), 7-chloroemodin and 7-chloro-1-O-methylemodin; the bianthrones and other anthraquinones were found to be inactive. Antiviral activity appeared to be pos. correlated with increasing substitution of chlorine in the anthraquinone structure. In the absence of light, only hypericin and 7,7'-dichlorohypericin displayed detectable activity.

IT **164397-06-2**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(antiviral activities of anthraquinones, bianthrones, and hypericin derivs. from lichens)

RN 164397-06-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dichloro-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

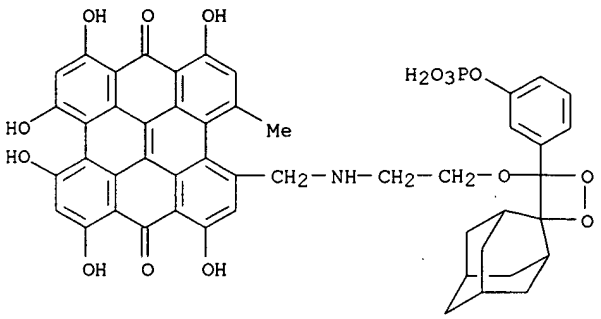


=> d bib abs hitstr l35 8

L35 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:826623 HCAPLUS
DN 123:237784
TI Inactivation of viruses present in blood components using chemically-activated compounds
IN Zepp, Charles M.; Heefner, Donald L.
PA Hemasure Inc., USA
SO PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

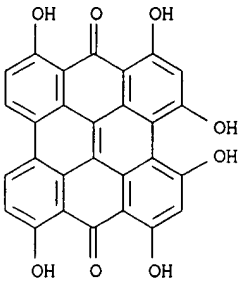
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9518530	A1	19950713	WO 1995-US464	19950109
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US				
	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2180854	AA	19950713	CA 1995-2180854	19950109
	AU 9515658	A1	19950801	AU 1995-15658	19950109
	EP 739163	A1	19961030	EP 1995-907419	19950109
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				

PRAI US 1994-179437 19940110
WO 1995-US464 19950109
OS MARPAT 123:237784
AB A method of inactivating viral mols. present within a blood sample and compds. for use in inactivation are described. The method involves adding to a virus-contg. blood sample an effective quantity of a compd. which both has an affinity for viral nucleic acid and which is activatable to an excited state in which the compd. covalently binds viral nucleic acid. After permitting the compd. to complex with viral nucleic acid, the compd. is raised to its excited state by chem. activation. Psoralen, hypericin or a deriv. of psoralen or hypericin is used as the activatable, viral-inactivating compd., and chem. activation of the compd. is effected by the decompn. of a dioxetane proximate to the nucleic acid/compd. complex. The activatable, viral-inactivating compd. is then orated into a dioxetane mol., and chem. activation of the compd. is effected by decompn. of the dioxetane into pair of carbonyl compds.
IT **168323-98-6**
RL: **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(inactivation of viruses in blood components using chem.-activated compds.)
RN 168323-98-6 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-methyl-11-[[[2-[[4-[3-(phosphonooxy)phenyl]spiro[1,2-dioxetane-3,2'-tricyclo[3.3.1.13,7]decan]-4-yl]oxy]ethyl]amino]methyl]- (9CI) (CA INDEX NAME)

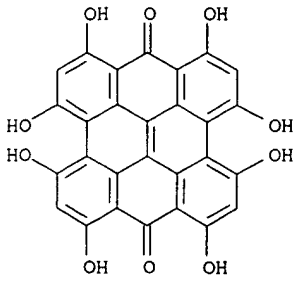

OH
O
OH
HO
HO
Me
H_2O_3PO
$CH_2-NH-CH_2-CH_2-O$
O
O
OH
O
OH

=> d bib abs hitstr l35 9

L35 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:615811 HCAPLUS
DN 123:65629
TI Hypericin as an inactivator of infectious viruses in blood components
AU Lavie, G.; Mazur, Y.; Lavie, D.; Prince, A.M.; Pascual, D.; Liebes, L.; Levin, B.; Meruelo, D.
CS Medical Center, New York University, New York, NY, USA
SO Transfusion (Bethesda, Md.) (1995), 35(5), 392-400
CODEN: TRANAT; ISSN: 0041-1132
DT Journal
LA English
AB Hypericin is a potent virucidal agent with activity against a broad range of enveloped viruses and retroviruses. The effective virucidal activity emanates from a combination of photodynamic and lipophilic properties. Hypericin binds cell membranes (and, by inference, virus membranes) and crosslinks virus capsid proteins. This action results in a loss of infectivity and an inability to retrieve the reverse transcriptase enzymic activity from the virion. Since hypericin is devoid of adverse action in most blood components and blood analyses, it is investigated as an additive with potential to inactivate infective viruses in blood components intended for transfusion. Complete inactivation of 106 tissue culture-IDs of human immunodeficiency virus was obtained in whole blood and in dild. packed red cells after illumination with fluorescent light for 1 h. Loss of viral infectivity to cultured CEM cells has been monitored by use of a detection assay for human immunodeficiency virus p55 in ELISA and cytopathic assays. In physiol. media, hypericin interacts with albumin and lipoproteins, retaining the virucidal activity in bound form. The mol. is neg. charged and forms org. and inorg. monobasic salts (ion pairs) in physiol. pH. Various ion pairs differ in virucidal efficacy. The apparent transfusibility of hypericin, taken together with the efficacy of the virucidal activity, the broad range of enveloped viruses affected, and the absence of adverse effects on stored red cells, may render hypericin useful for inactivation of infectious viruses in red cells.
IT **60935-17-3**, Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy- **157301-83-2**
RL: BAC (Biological activity or effector, except adverse); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(hypericin and analogs for virus inactivation in blood preservation)
RN 60935-17-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy- (9CI) (CA INDEX NAME)



RN 157301-83-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy- (9CI) (CA INDEX NAME)

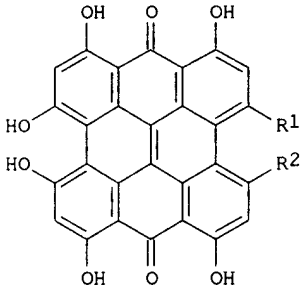

OH
O
OH
HO
OH
HO
OH
OH
O
OH

=> d bib abs hitstr l35 10

L35 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:354447 HCAPLUS
DN 122:132851
TI Preparation of hypericin dicarboxylate esters as antiviral agents
IN Mazur, Yehuda; Lavie, Gad; Meruelo, Daniel; Lavie, David
PA Yeda Research and Development Co., Ltd., Israel; New York University
SO PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9427952	A1	19941208	WO 1994-US5975	19940527
	W: AU, CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9472023	A1	19941220	AU 1994-72023	19940527
	AU 689120	B2	19980326		
	EP 702669	A1	19960327	EP 1994-921214	19940527
	EP 702669	B1	19980729		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 08510753	T2	19961112	JP 1994-500974	19940527
	AT 168985	E	19980815	AT 1994-921214	19940527
	IL 109807	A1	19981206	IL 1994-109807	19940527
	ES 2122303	T3	19981216	ES 1994-921214	19940527
PRAI	US 1993-68379		19930527		
	WO 1994-US5975		19940527		

OS MARPAT 122:132851
GI

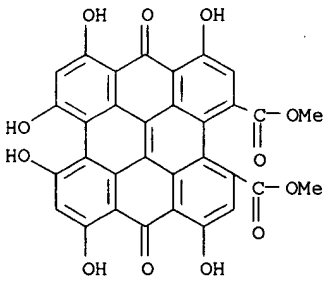


I

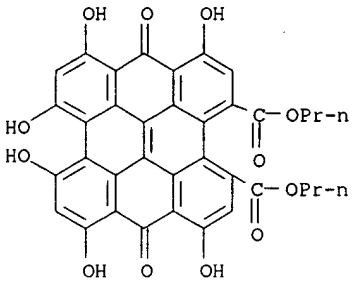
AB Title compds. I (R1, R2 = alkyl, R3O2C wherein R3 = alkyl, the chain of which is optionally interrupted by one or more O, S, and at least 1 of R1 and R2 is R3O2C). Emodic acid anthrone in MeOH contg. H2SO4 was refluxed for 4 h to give emodic acid anthrone Me ester which in pyridine and piperidine to which was added pyridine N-oxide and FeSO4.7H2O were refluxed for 3 h at 100.degree. to give after workup I (R1 = R2 = MeO2C). Virucidal activity was demonstrated. Pharmaceutical compns. are claimed (no data).

IT **160919-80-2P 160919-81-3P 160919-82-4P**
160919-83-5P 160919-84-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of hypericin dicarboxylate esters as antiviral agents)

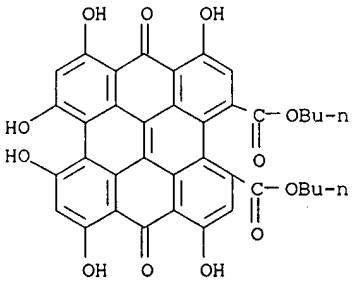
RN 160919-80-2 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, dimethyl ester (9CI) (CA INDEX NAME)



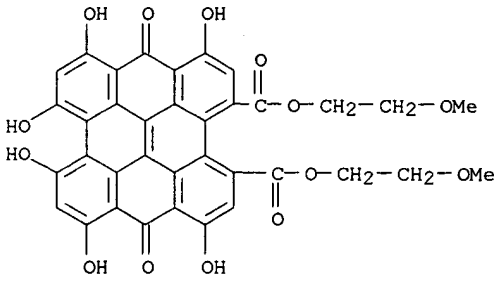
RN 160919-81-3 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, dipropyl ester (9CI) (CA INDEX NAME)



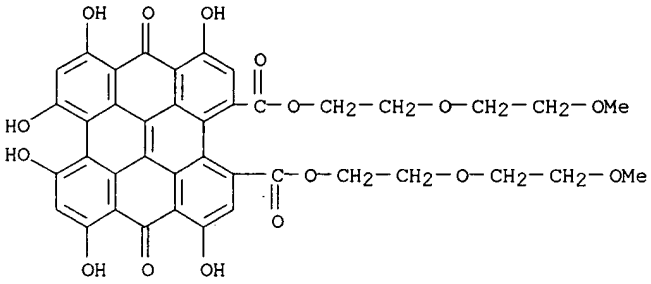
RN 160919-82-4 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, dibutyl ester (9CI) (CA INDEX NAME)



RN 160919-83-5 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, bis(2-methoxyethyl) ester (9CI) (CA INDEX NAME)



RN 160919-84-6 HCAPLUS
CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, bis[2-(2-methoxyethoxy)ethyl] ester (9CI) (CA INDEX NAME)



```
=> d bib abs hitstr 135 11

     10 ANSWERS ARE AVAILABLE.  SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE
The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):end
```